PROCEEDINGS OF SIMAI 2016

THE XIII BIANNUAL CONGRESS OF SIMAI

13-16 SEPTEMBER 2016

MILAN, ITALY

Editors: L. Bonaventura, L. Formaggia, E. Miglio, N. Parolini, A. Scotti and C. Vergara

SIMAI
SOCIETÀ ITALIANA DI MATEMATICA APPLICATA E INDUSTRIALE

Conference logo design by Anna Scotti. Typographic composition made in LaTeX by Mattia Penati.

SIMAI
SOCIETÀ ITALIANA DI MATEMATICA APPLICATA E INDUSTRIALE
http://www.simai.eu

ISBN 978-88-6493-035-0

Preface

Since 1992, the Italian Society for Applied and Industrial Mathematics (SIMAI) holds a biennial congress gathering contributions of researchers from academia and industry working on industrial and applied mathematics problems.
This book collects the abstracts of the talks and plenary lectures given at the SIMAI Congress 2016 that took place in Milano, Italy, from September 13 to September 16, 2016.
We are extremely satisfied that so many people have shown their interest in this meeting. In addition to 6 invited plenary lectures, we had more than 360 contributions from Italy and many other European countries, organized into 64 minisymposia. The contributions contained in this book cover both theoretical aspects and practical applications of mathematics and scientific computing. Topics include the analysis of evolution and dissipative processes, stochastic modeling, numerical methodologies such as computational optimization, advanced numerical methods for PDEs, conservation laws and inverse problems, optimal control, model reduction and high-performance-computing, as well as statistical methodologies for the treatment of complex data and signals.
A wide range of applications is covered from life science and biology to geophysics, from image processing to petroleum engineering and quantitative finance.
We would like to thank all participants for their valuable contributions. In particular we mention the fundamental contribution of the minisymposia organizers.
Special thanks are due to the invited speakers: P. Antonietti (Politecnico di Milano), A. Buffa (IMATI-CNR), A. Pontremoli (Dallara Automobili), Wil Schilders (TU Eindhoven), A. Quarteroni (EPFL), and G. Toscani (University of Pavia), for contributing to the success of the conference with the high quality of their contributions.
We gratefully acknowledge the support of the industrial sponsors: Mathesia, MOXOFF, Noesis and SpingerNature.
Finally we would like to thank the Politecnico di Milano for hosting the Congress and, in particular, the Eventimate Team (Anna Rho and Laura Guarino) for the logistic support in the organization of the conference and Luca Lo Curto for the technical support. Moreover we thank and all volunteers (mainly post-doc and PhD students) for their help during the meeting.
We believe that the wide range of applications and the scientific quality of the contributions collected in this book represent the best evidence of the important role that the industrial and applied mathematics can play in our society.
We believe that this book gives an up-to-date description of the state of the art of the research in industrial and applied mathematics in Italy.

Milano, Italy
September 2016

The Organizing Committee

Back to Table of Contents

Contents

Individual contributions

Minisymposia

Plenaries

Individual contributions

Boundary stabilization of a flexible beam with a tip rigid body without dissipativity

Moulay Driss Aouragh
FST. Moulay Ismail University, M2I laboratory, MAMCS Group,
Comp. sciences Dept. B.O. BOX 509, Boutalamine, Errachidia-Morocco
d.aouragh@fste.umi.ac.ma

Abderrahman El Boukili
FST. Moulay Ismail University, M2I laboratory,
B.O. BOX 509, Boutalamine, Errachidia-Morocco
aelboukili@gmail.com

A linear feedback control is designed regardless of dissipativity of the system of a flexible structure modeled by an Euler-Bernoulli beam which is held by a rigid hub at one end and totally free at the other [1].To realize the uniform stabilization, the high derivative feedback control is usually required. However, on the other hand, the design of the high derivative feedback controllers in literature are mainly based on principle of passivity that makes the closed-loop system be dissipative so that the system is at least asymptotically stable by lyapunov function method. In applications, on the other hand, there are many ways of designing controllers that make system pratically uniformly stable but there is no dissipativity which usually brings the difficulty of theoretical proof for the uniform stability of the system. The approach used here is so called Riesz basis approach [2] that is recently used to study the basis generation, exponential stability and distribution of eigenvalues of the Euler-Bernoulli beam equations.

References

[1] Fukuda T., Kuribayashi Y, Hosogai H. and Yajima N.,1985 *Vibration mode estimation and control of flexible solar battery arrays on solar cell outputs.* Theoret. Appli. Mech. 33, 299–309.

[2] Guo B. Z. and Yu R., 2001 *The Riesz basis property of discrete operators and application to a Euler-Bernoulli beam equation with boundary linear feedback control* IMA J. of Math. Control and Information, 18, 241–251.

Modeling spatio-temporal functional data with complex dependencies via regression with partial differential regularizations

Mara S. Bernardi
MOX - Dipartimento di Matematica, Politecnico di Milano
Piazza Leonardo da Vinci 32, 20133 - Milano, Italy
marasabina.bernardi@polimi.it

Gabriele Mazza
MOX - Dipartimento di Matematica, Politecnico di Milano
Piazza Leonardo da Vinci 32, 20133 - Milano, Italy
gabriele.mazza@mail.polimi.it

Laura M. Sangalli
MOX - Dipartimento di Matematica, Politecnico di Milano
Piazza Leonardo da Vinci 32, 20133 - Milano, Italy
laura.sangalli@polimi.it

James O. Ramsay
Department of Psychology, Mc Gill University
845 Sherbrooke Street West, H3A 0G4 - Montreal, Quebec, Canada
james.ramsay@mcgill.ca

We present the model introduced in [1] for the analysis of functional data with complex dependencies, such as spatially dependent curves or time dependent surfaces. The model is based on the idea of regression with partial differential regularizations. Among the various modeling features, the proposed method is able to deal with spatial domains featuring peninsulas, islands and other complex geometries. Space-varying covariate information is included in the models via a semiparametric framework. The estimators have a penalized regression form, they are linear in the observed data values, and have good inferential properties. The use of numerical analysis techniques, and specifically of finite elements, makes the models computationally very efficient. The model is compared via simulations to other spatio-temporal techniques and it is illustrated via an application to the study of the annual production of waste in the municipalities of Venice province.

References

[1] M. S. Bernardi, L.M. Sangalli, G. Mazza, J. O. Ramsay, *A penalized regression model for spatial functional data with application to the analysis of the production of waste in Venice province*, Stochastic Environmental Research and Risk Assessment, DOI: 10.1007/s00477-016-1237-3

Heat rectification and thermal wave propagation in graded materials

Isabella Carlomagno
University of Basilicata
Department of Mathematics, Computer Science and Economics
Viale dell'Ateneo Lucano 10 85100- Potenza Italy
isabellacarlomagno85@gmail.com

Vito Antonio Cimmelli
University of Basilicata
Department of Mathematics, Computer Science and Economics
Viale dell'Ateneo Lucano 10 85100 - Potenza Italy
vito.cimmelli@unibas.it

David Jou
Universitat Autònoma de Barcelona
Department of Physics
08193 - Bellaterra, Catalonia Spain
david.jou@uab.es

We investigate the effects of a composition gradient and of a non vanishing heat flux on the phase speed of thermal waves propagating along a graded system. To this end, we apply a generalized heat-transport equation which is capable to account for non-local and non-linear effects [4]. The results for high-frequency and low-frequency waves are compared. For low frequency, we discuss the conditions in which thermal waves may propagate in Si_xGe_{1-x} and $(Bi_{1-x}Sb_x)_2Te_3$ alloys, with x a suitable stoichiometric variable accounting for the variation of the composition along a given direction [2]. We also calculate the heat rectification coefficient of a composition-graded system of the type $\mathrm{A}_x\,\mathrm{B}_{1-x}$, with A and B theoretical materials, and composition x changing along the length of the system. The influence of composition spatial distribution, heat flux, length of the system, and minimum of thermal conductivity on the rectification coefficient is pointed out. It is observed a reversal in the direction of the rectification for increasing heat flux [1]. Finally, we study propagation of low-frequency thermal waves in graded Si_xGe_{1-x}, and show that in some ranges of stoichiometry variation one obtains rectification of thermal waves, i.e., the system allows the propagation of waves in one direction but not in the opposite one through the graded system, or through a thin graded layer separating two different systems [3].

References

[1] Carlomagno, I., Cimmelli,V. A. and Jou, D. 2016 *Computational analysis of heat rectification in composition-graded systems: From macro-to-nanoscale* Physica B 481, 244–251.

[2] Jou, D., Carlomagno, I. and Cimmelli,V. A. 2015 *A thermodynamic model for heat transport and thermal wave propagation in graded systems* Physica E 73, 242–249.

[3] Jou, D., Carlomagno, I. and Cimmelli,V. A. 2016 *Rectification of low-frequency thermal waves in graded* Si_cGe_{1-c} Physics Letters A. In press.

[4] Sellitto, A., Cimmelli, V. A. and Jou, D. 2016 *Mesoscopic theories of heat transport in nanosystems*. Berlin: Springer.

Non-Fourier heat transfer with phonons and electrons in circular thin layers

Vito Antonio Cimmelli
University of Basilicata
Department of Mathematics, Computer Science and Economics
Viale dell'Ateneo Lucano 10 - 85100 - Potenza, Italy
vito.cimmelli@unibas.it

Isabella Carlomagno
University of Basilicata
Department of Mathematics, Computer Science and Economics
Viale dell'Ateneo Lucano 10 - 85100 - Potenza, Italy
isabellacarlomagno85@gmail.com

Antonio Sellitto
University of Salerno
Department of Industrial Engineering
Via Giovanni Paolo II, 132 - 84084 - Fisciano, Italy
ant.sellitto@gmail.com

A nonlocal model for heat transfer with phonons and electrons is applied to infer the steady-state radial temperature profile in a circular layer surrounding a inner hot component [6]. Such a profile, following by the numerical solution of the heat equation, predicts that the temperature behaves in an anomalous way, since for radial distances from the heat source smaller than the mean-free paths of phonons and electrons it increases with the radial distance [2].
The previous analysis is extended to a semi-metallic thin layer [1], which allows for different temperatures of phonons and electrons [3, 4]. Also in this case, the model predicts that in some range of distances from the heat source the temperature increases for increasing radial distances.
In both the situations considered above, the compatibility of this nonstandard temperature behavior with the second law of thermodynamics is investigated in view of the requirement of positive entropy production and of a nonlocal constitutive equation for the entropy flux [5]. It is shown that such a situation does not conflict with the restrictions imposed by second law of thermodynamics [1, 2].

References

[1] Carlomagno, I., Cimmelli, V. A. and Sellitto, A. 2016 *Heat conduction with phonons and electrons in two-dimensional semimetals*. Submitted.

[2] Cimmelli,V. A., Carlomagno, I. and Sellitto, A. 2015 *Non-Fourier Heat Transfer with Phonons and Electrons in a Circular Thin Layer Surrounding a Hot Nanodevice* Entropy 17, 5157–5170.

[3] Jou, D., Sellitto, A. and Cimmelli, V. A. 2013 *Phonon temperature and electron temperature in thermoelectric coupling*. J. Non-Equilib. Thermodyn. 38, 335–361.

[4] Jou, D., Sellitto, A. and Cimmelli, V. A. 2014 *Multi-temperature mixture of phonons and electrons and nonlocal thermoelectric transport in thin layers*. Int. J. Heat Mass Transfer 71 459–468.

[5] Sellitto, A., Cimmelli, V. A. and Jou, D. 2016 *Mesoscopic theories of heat transport in nanosystems*. Berlin: Springer.

[6] Sellitto, A., Cimmelli, V. A. and Jou, D. 2013 *Entropy flux and anomalous axial heat transport at the nanoscale*. Phys. Rev. B 87, 054302-1 – 054302-7.

Approximation by max-product neural network operators activated by sigmoidal functions

Danilo Costarelli
Università degli Studi di Perugia
via Vanvitelli, 1 06123 - Perugia Italy
danilo.costarelli@unipg.it

Gianluca Vinti
Università degli Studi di Perugia
via Vanvitelli, 1 06123 - Perugia Italy
gianluca.vinti@unipg.it

The theory of neural network (NN) operators (see e.g., [1, 2]) has been introduced and studied in lasts fifteen years, and it is strictly related to the classical theory of artificial neural networks (NNs), see e.g., [4]. The NNs have been introduced in 1900's in order to construct a simple model for the human brain, which is able to represent all its main abilities. From a mathematical point of view, NNs are defined by finite linear combination of sigmoidal activation functions, suitably shifted and scaled by certain coefficients, weights and thresholds. The high number of parameters composing a NN makes this kind of tools very flexible, hence very useful for the applications in Approximation Theory, and in many other fields.

The definition of the max-product NN operators has been introduced in [1], and has been successively extended in [3]. Such families of nonlinear operators (more precisely sublinear), allow us to approximate functions of one and several variables, by a constructive formula, and with an higher order of approximation with respect to their corresponding classical (linear) counterparts, studied in [2]. In [3], some estimate concerning the rate of convergence for the max-product NN operators have been proved employing the modulus of continuity of the functions being approximated. Moreover, a comparison with the results proved in [1, 2] is given. Finally, several examples of sigmoidal activation functions for which the above theory can be applied are given, together with some numerical examples for the approximation process studied.

References

[1] Anastassiou, G.A., Coroianu, L. and Gal, S.G. 2010 *Approximation by a nonlinear Cardaliaguet-Euvrard neural network operator of max-product kind*, J. Comp. Anal. Appl. 12 (2), 396–406.

[2] Costarelli, D. and Spigler, R. 2013 *Approximation results for neural network operators activated by sigmoidal functions*. Neural Networks. 44, 101–106.

[3] Costarelli, D. and Vinti, G. 2015 *Max-product neural network and quasi-interpolation operators activated by sigmoidal functions*, submitted to J. Approx. Theory.

[4] Cybenko, G 1989 *Approximation by superpositions of a sigmoidal function*, Math. Control Signals Systems. 2, 303–314.

Multi scale modelling and model reduction for lithium-ion batteries

Matteo Icardi
University of Warwick
Mathematics Institute, CV4 7AL – Coventry, UK
matteo.icardi@warwick.ac.uk

Florian Theil
University of Warwick
Mathematics Institute, CV4 7AL – Coventry, UK
f.theil@warwick.ac.uk

Lithium-ion batteries present many modelling challenges, including complex electrochemical reaction, transport in porous materials, multi-scale random heterogeneous structure. Several approaches have been developed to describe and numerically solve micro- or meso-scale equations. However, for practical applications such as hybrid vehicles, there is an increasing need of fast online, yet accurate, simple reduced models. State-of-the-art macroscopic models for battery applications are defined by system identification techniques and fail to capture the intrinsic functional dependence of the parameters on the material attributes and to predict irreversible and complex non-linear phenomena such as fast (dis)charge and degradation. We present an analytical approach for model reduction, based on spectral analysis of the underlying PDEs, to develop simple and efficient reduced order models, as an alternative to classical equivalent circuit models. Starting from the well-know porous electrode theory and Newman's model, we derive and solve simple differential equations that can retain the interesting features of the full model (e.g., solid diffusion, non-linearities). This model can easily be implemented in online battery management systems and can be coupled with advanced data-assimilation techniques. We also discuss the possibility of a full multi-scale approach by integrating pore-scale analysis of the porous micro-structures via fully resolved direct numerical simulations.

References

[1] Icardi, M., Boccardo, G., Marchisio, D. L., Tosco, T., & Sethi, R. (2014). Pore-scale simulation of fluid flow and solute dispersion in three-dimensional porous media. *Physical Review E*, 90(1), 013032.

[2] Newman, J., & Tiedemann, W. (1975). Porous-electrode theory with battery applications. *AIChE Journal*, 21(1), 25-41.

[3] Latz, A., Zausch, J., & Iliev, O. (2010). Modeling of species and charge transport in li–ion batteries based on non-equilibrium thermodynamics, in *Numerical Methods and Applications* (pp. 329-337), Lecture Notes in Computer Science, vol 6046. Springer Berlin Heidelberg.

[4] Icardi, M. & Theil, F. (in preparation). PDE-based model reduction and multi-scale simulation for lithium-ion batteries.

Oxygen transport in the eye retina tissue: mathematical and computational modeling

Francesca Malgaroli
Dipartimento di Matematica, Politecnico di Milano
piazza Leonardo da Vinci, 32 20133 - Milano Italy
francesca.malgaroli@polimi.it

Paola Causin
Dipartimento di Matematica, Università degli Studi di Milano
via C. Saldini, 50 20133 - Milano Italy
paola.causin@unimi.it

Martina Geroli
Dipartimento di Matematica, Università degli Studi di Milano
via C. Saldini, 50 20133 - Milano Italy
paola.causin@unimi.it

The retina is a complex matrix of neural cells lining the innermost surface of the eye globe. Light travels through its thickness before striking and activating the photoreceptors and the visual information is then relied to the brain by nerve bundles. The different neural cells present in the retina have highly stratified oxygen consumption rates, so that a "metabolic compartmentalization" can be identified. It is customary to distinguish two main retinal regions: *i)* the outer retina (OR), containing photoreceptor mitochondria, proximal to the sclera, avascular and nourished in oxygen by diffusion from the large pool represented by the choroidal circulation; *ii)* the inner retina (IR), proximal to the vitreous and nourished in oxygen by the embedded microcirculatory network.

In this work, we propose a mathematical model to study the oxygen pressure profile along the retinal depth. Our aim is to compute an analytic solution for the oxygen profile and use it to perform a sensitivity analysis study. Following several models in literature (see *e.g.* [3]), we adopt a subdivision of the OR into three layers (denoted by 1,2,3 respectively), while we represent the IR as a single layer (layer 4), ending up with a model partitioned in four layers. The phenomena we include are oxygen diffusion through the tissue, which is modeled with a constant diffusivity coefficient D [cm^2/s] along all the depth and reaction/source terms. Letting $z \in [0, L_t]$ be the coordinate along the retinal thickness, we set $\Omega = (0, L_t)$ and we denote by $\Omega_j, j = 1, \dots, 4$, such that $\Omega = \bigcup_{j=1,\dots,4} \Omega_j$, the subdomains representing the four layers. The resulting model, upon averaging in the plane orthogonal to the retina thickness, yields the following 1D problem: find the oxygen tension p [mmHg] such that

$$\begin{cases} -D\dfrac{\partial^2 p}{\partial z^2} = S(p, p_c) - C(p) \quad \text{in } \Omega, \\ p(z=0) = p_{ch}, \qquad D\dfrac{\partial p}{\partial z}|_{z=L_t} = 0, \end{cases} \tag{1}$$

where p_{ch} is the prescribed source from the choroid, S is the distributed oxygen source from blood circulation (with blood oxygen tension p_c) and C the metabolic consumption

term. The source and consumptions terms are given by:

$$S(p, p_c) = \begin{cases} 0 & \text{in} \quad \Omega_1, \Omega_2, \Omega_3, \\ f & \text{in} \quad \Omega_4, \end{cases}$$

f being a prescribed constant, and

$$C(p) = \begin{cases} q & \text{in} \quad \Omega_1, \Omega_3, \Omega_4, \\ Q^{\max} \dfrac{p}{p + k_{0.5}} & \text{in} \quad \Omega_2, \end{cases}$$

where q is a prescribed constant ($q = 0$ in Ω_1, Ω_3) and where the nonlinear Michaelis-Menten kinetics is used to model consumption in layer 2 (photoreceptor metabolism), $Q^{\max}$ being the maximal consumption rate and $k_{0.5}$ the oxygen pressure at half maximal consumption rate.

According to the model assumptions, it is straightforward to find the solutions in layers 1, 3 (linear functions) and 4 (parabolic function). In layer 2 of the OR, we find an approximate analytical solution of the nonlinear diffusion-reaction problem by the so-called *homotopy perturbation method* (see [2] for a basic introduction to the method and [4] for an application similar to the one of this work). The resulting analytic expressions of $p = p(z)$ in the different layers, depend parametrically on a set of constants which are saturated by joining adjacent layers. This is done by imposing the continuity of oxygen tension and oxygen flux. By doing this, we end up with a system of three equations in three unknowns (representing oxygen tensions at the interfaces between layers 1 and 2, 2 and 3, 3 and 4, respectively). The resolution of such a system, which is onerous due to the complexity of the solution in layer 2, is faced with the symbolic engine of MATLAB®.

We use the analytical expression of the total oxygen pressure profile to carry out a sensitivity study by computing the derivatives of the solution with respect to different parameters. Due to the complexity of the expressions, we perform such an analysis on two simplified models, obtained merging layers of the OR. Sensitivity results evidence that the reaction term in IR is the parameter to which the oxygen profile is most sensitive. As a matter of fact, the shape of the pressure profile is governed by the sign and value of $S(p, p_c) - C(p)$ in the IR. This finding agrees with the experimental evidence of the delicate balance of oxygen supply-to-consumption existing in this region and with the clinical knowledge of the fact that impaired retinal circulation is a main determinant of retinal tissue pathologies.

References

[1] Causin, P., Guidoboni, G., Malgaroli, F., Sacco, R., Harris, A. (2015). *Blood flow mechanics and oxygen transport and delivery in the retinal microcirculation: multiscale mathematical modeling and numerical simulation.* Biomechanics and modeling in mechanobiology, 1-18.

[2] Babolian, E., Azizi, A., Saeidian, J. (2009). *Some notes on using the homotopy perturbation method for solving time-dependent differential equations.* Mathematical and Computer Modelling, 50(1), 213-224.

[3] Birol, G., Wang, S., Budzynski, E., Wangsa-Wirawan, N. D., Linsenmeier, R. A. (2007). *Oxygen distribution and consumption in the macaque retina.* American Journal of Physiology-Heart and Circulatory Physiology, 293(3), H1696-H1704.

[4] Shanthi, D., Ananthaswamy, V., Rajendran, L. (2013). *Analysis of non-linear reaction-diffusion processes with Michaelis-Menten kinetics by a new Homotopy perturbation method.* Natural Science, 5(09), 1034.

Computationally enhanced projection methods for symmetric Lyapunov matrix equations

Davide Palitta
Dipartimento di Matematica, Università degli Studi di Bologna
P.zza di Porta S. Donato, 5 40126 - Bologna Italy
davide.palitta3@unibo.it

Valeria Simoncini
Dipartimento di Matematica, Università degli Studi di Bologna
P.zza di Porta S. Donato, 5 40126 - Bologna Italy
valeria.simoncini@unibo.it

In the numerical treatment of large-scale Lyapunov equations, projection methods require solving a reduced Lyapunov problem to check convergence. As the approximation space expands, this solution takes an increasing portion of the overall computational effort. When data are symmetric, we show that the Frobenius norm of the residual matrix can be computed at significantly lower cost than with available methods, without explicitly solving the reduced problem. For certain classes of problems, the new residual norm expression combined with a memory-reducing device make classical Krylov strategies competitive with respect to more recent projection methods. In this talk, we present several numerical experiments that illustrate the effectiveness of the new implementation for standard and extended Krylov subspace methods.

References

[1] Palitta, D. and Simoncini, V., *Computationally enhanced projection methods for symmetric Sylvester and Lyapunov equations.* ArXiv: 1602.05033.

Nonlinear elasto-plasticity for finite-strain deformations

Roberto Porcù
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
roberto.porcu@polimi.it

Edie Miglio
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
edie.miglio@polimi.it

Mattia Penati
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
mattia.penati@polimi.it

The aim of this work is the numerical simulation of continental rifting processes, motivated by the fact that these geological phenomena play a very relevant role in geodynamics investigations. In this sense a good portion of the research currently done about this topic by scientists consists in the analysis of analogical models, named sandbox, which try to reproduce the real behavior of the rifting phenomena. The development of a *numerical sandbox*, that was the objective of this work, is explained by the several issues inherent to the analogic experiments: they are expensive, they are extremely simplified, their results are mostly qualitative. The constitutive laws that control the motion of the numerical sandbox are described by a fully-nonlinear elasto-plastic rheology which is best suited for finite-strain deformations. The motion is described in a Lagrangian way since the spatial physical quantities that represent the variables of the problem are parametrized on the reference configuration. Thanks to the nondimensionalization of the equations a quasi-static motion is assumed. For the numerical discretization a three-field variational formulation of the problem has been taken into account in order to prevent the volumetric locking arising from the enforcement of a nearly isochoric deformation, as stated in [1]: an independent volume field is introduced together with its dual variable that can be interpreted as the Kirchhoff pressure. This leads to an additive decomposition of the Helmoltz free energy into its isochoric and volumetric parts. The implicit update of the state of the system is computed by means of the Newton-Raphson method. Using the Kröner-Lee decomposition, the deformation gradient is multiplicatively decomposed into its elastic and plastic parts. The constitutive update is computed point-wise on the spatial quadrature nodes: an elastic trial is firstly computed; if the trial deformation lies outside the elastic domain then the plastic exponential return map brings the nodal deformation back on the boundary of the elastic domain. A Drücker-Prager yield failure criterion and a non-associative flow rule have been considered since these are really good choices for geological applications, as stated in [2]. The developed code is written in C++, it is based on the deal.II finite element library, it works in parallel by means of the MPI

and multi-threading paradigms, it handles three-dimensional geometries. The results show the natural formation of shear bands with a V-pattern that the most-diffused softwares for geodynamics simulations are able to catch only if a weak seed is artificially added into the domain.

References

[1] Simo, J. C. 1998 Numerical analysis and simulation of plasticity. In *Handbook of Numerical Analysis*, 6, 183–499. Elsevier.

[2] Belytschko, T. and Liu, W. K. and Moran, B. 2001 Nonlinear Finite Elements for Continua and Structures. Wiley.

Decay bounds for functions of structured non-Hermitian matrices

Stefano Pozza
Università di Bologna
Piazza di Porta S. Donato, 5 40127 - Bologna - Italy
stefano.pozza@unibo.it

Valeria Simoncini
Università di Bologna
Piazza di Porta S. Donato, 5 40127 - Bologna - Italy
valeria.simoncini@unibo.it

The derivation of decay bounds for the entries of functions of matrices has attracted the interest of many researchers working in a wide range of applications, such as numerical analysis, harmonic analysis, quantum chemistry, signal processing, quantum information theory, multivariate statistics, queuing models, control of large-scale dynamical systems, quantum dynamics, random matrix theory, and others; see [1] and references therein. While decay bounds for functions of Hermitian banded matrices have been known for some time, only recently more structured sparsity patterns have been analyzed. Moreover, the non-Hermitian case is an especially challenging setting. By using Faber polynomial series we first extend results for Hermitian matrices to banded non-Hermitian matrices. We then describe the limitations of this approach in capturing the true decay in certain situations. Hence, we derive new bounds that accurately describe the decay behavior of Cauchy-Stieltjes functions of real non-Hermitian banded matrices. These results are then generalized to Kronecker sums of banded matrices.

This talk is based on current work in progress [2].

References

[1] Benzi, M. and Simoncini, V. 2015 *Decay bounds for functions of hermitian matrices with banded or kronecker structure*. SIAM J. Matrix Anal. Appl. 36(3), 1263–1282.

[2] Pozza, S. and Simoncini, V. 2016 *Decay bounds for functions of structured non-hermitian matrices*. in preparation.

Recent results on scattering coefficients for the Stochastic Nonlinear Schroedinger Equation

Laura Prati
Università degli Studi di Firenze
via S.Marta, 3 50139 - Firenze Italy
laura.prati@unifi.it

Luigi Barletti
Università degli Studi di Firenze
Viale Morgagni, 67/a 50134 - Firenze Italy
luigi.barletti@unifi.it

The demand for telecommunication services has become increasingly urgent over the years, making the existing networks and infrastructure inadequate. In the late Seventies, the fiber-optic communications were introduced causing great progress of technological nature that allowed to exponentially increase the data traffic. The Nonlinear Schroedinger Equation governs the evolution of the complex envelope of signals propagating in optical fibers. The stochastic version of the Nonlinear Schroedinger Equation also introduces the presence of optical noise, which is added to non-linear effects of propagation along the fiber. For a single-mode fiber, the stochastic Nonlinear Schroedinger Equation in case of anomalous dispersion (focusing fiber) is

$$\frac{\partial q}{\partial z}(z,t) = \frac{i}{2}\frac{\partial^2 q}{\partial t^2}(z,t) + iq(z,t)|q(z,t)|^2 + \eta(z,t)$$

where $q(z,t)$ is the complex field envelope, z is the normalized distance along the fiber, t is time in a frame moving with the the group velocity of the envelope, i is the imaginary unit and $\eta(z,t)$ is the additive white Gaussian noise having zero mean.

The strong distortion of the optical signal makes it difficult to decode the information at the receiver (possibly located tens of kilometers away from the transmitter) and limits the transmission rate of the information itself. By referring to the Nonlinear Fourier Transform approach, used to treat exactly solvable nonlinear partial differential equations (as the deterministic Nonlinear Schroedinger Equation), nowadays the idea is to transmit information by encoding it not directly on the optical signal, but on the nonlinear spectrum associated with it. The forward Nonlinear Fourier Transform operation maps the initial envelope onto a set of scattering coefficients, related to both the discrete and the continuous spectrum. We focus on the behavior of the scattering coefficients along the propagation in order to understand and describe their statistics and, as a direct consequence, the properties of the channel. The comprehension of the non deterministic terms lays the foundation for understanding the influence of noise on the received spectra. We assume that the signal-to-noise ratio is high (η small) and we use a perturbation approach in order to determine the hierarchy of perturbation equations for the propagation of eigenvalues and scattering data. The zero-order perturbation leads to the deterministic Nonlinear Schroedinger Equation.

On the efficiency of thermoelectric energy conversion

Patrizia Rogolino
Università degli Studi di Messina
Viale G. Stagno D'Alcontres, 98166 - Messina Italy
progolino@unime.it

Vito Antonio Cimmelli
University of Basilicata
Department of Mathematics, Computer Science and Economics
Viale dell'Ateneo Lucano 10 - 85100 - Potenza, Italy
vito.cimmelli@unibas.it

Antonio Sellitto
University of Salerno
Department of Industrial Engineering
Via Giovanni Paolo II, 132 - 84084 - Fisciano, Italy
ant.sellitto@gmail.com

The relation between the thermodynamic efficiency in thermoelectric coupling and the breakdown of the Onsager Symmetry (OS) [1] in nonlinear regime is pointed out. Some practical examples in which the OS is lost are analyzed, proving that this is due to the presence of nonlinear terms in the evolution equation for the heat flux [2]. Moreover, it is seen that, due to the breakdown of the OS, the Second Kelvin Relation [1, 5] of classical thermoelectricity changes in a more general expression, which is capable to influence the efficiency of thermoelectric coupling [2, 3]. It is also shown that the presence of a non homogeneous electric-charge distribution inside the conductor contributes to a reduction of the efficiency, since the motion of free charges results in an additional energy dissipation by Joule effect [4].

References

[1] Lebon, G. , Jou, D. and Casas-Vázquez, J. 2008 *Understanding nonequilibrium thermodynamics*. Berlin: Springer.

[2] Rogolino, P., Sellitto, A. and Cimmelli, V. A. 2015 *Influence of nonlinear effects on the efficiency of a thermoelectric generator*. Z. Angew. Math. Phys., vol. DOI:10.1007/s00033-015-0516-z, p. in press.

[3] Rogolino, P., Sellitto, A. and Cimmelli, V. A. 2015 *Influence of the electron and phonon temperature and of theelectric-charge density on the optimal efficiency of thermoelectricnanowires*. Mechanics Research Communications, p. in press.

[4] Rogolino, P., Sellitto, A. and Cimmelli,V. A. *A nonlinear model of thermoelectricity with two temperatures: Application to quasicrystalline nanowires*. Submitted.

[5] Sellitto, A., Cimmelli, V. A. and Jou, D. 2016 *Mesoscopic theories of heat transport in nanosystems*. Berlin: Springer.

A Local Adaptive Method for the Numerical Approximation of Seismic Inversion Problems

Bruno Giovanni Galuzzi
Università degli Studi di Milano
via Festa del Perdono, 7 20122 - Milano Italy
bruno.galuzzi@unimi.it

Elena Zampieri
Università degli Studi di Milano
via Festa del Perdono, 7 20122 - Milano Italy
elena.zampieri@unimi.it

Eusebio Maria Stucchi
Università degli Studi di Milano
via Festa del Perdono, 7 20122 - Milano Italy
eusebio.stucchi@unimi.it

The seismic wave propagation in a geological medium is often modelled by the acoustic $2D$ equation

$$\ddot{p} = c(x,z)^2 \Delta p + \delta(x - x_0)\delta(z - z_0)s(t),$$

where p is the pressure of the wave, c is the velocity, and $s(t)$ is the seismic wavelet, describing the variation of the seismic source in time.
Building an accurate numerical implementation of this equation is very important in the framework of Full Waveform Inversion, a classical contest of data inversion in which the numerical solution of the wave equation is compared with one or more seismograms in order to obtain information on the Earth's subsurface [3].
If we use a finite difference grid to approximate the space domain, the approximation error depends on the space step dx and the order of approximation of spatial derivatives p. Generally, the main relation that links these two parameters with the physical parameters is the numerical dispersion inequality

$$dx < \frac{c_{min}}{f_{max}\, n},$$

where $n = n(p)$ is the number of points per wavelength, c_{min} is the minimum velocity of the model and f_{max} is the maximum frequency of the source signal $s(t)$ [1].

Using the same order of approximation for all the grid points reduce the efficiency, because numerical dispersion is a local phenomenon that depends on the local velocity, while the numerical dispersion relation refers to the minimum velocity in the whole spatial domain.
In this work we describe a new numerical approach for the solution of the acoustic wave equation that optimizes the numerical dispersion relation on the basis of the local velocity of the grid nodes. In particular, the order of approximation of the spatial derivatives for a grid node is chosen as a function of a local numerical dispersion inequality

$$dx < \frac{c_{loc}}{f_{max}\, n_{loc}},$$

where c_{loc} is the local velocity of the grid node and $n_{loc} = n_{loc}(p_{loc})$ is the number of points per local wavelength which is a function of the local order.
As an example of application Fig.1a and Fig.1b show the velocity model (a readjustment of a portion of the Marmousi model [2]) and the source-receiver layout used to simulate a seismic acquisition, respectively. In the numerical implementation we consider a recording

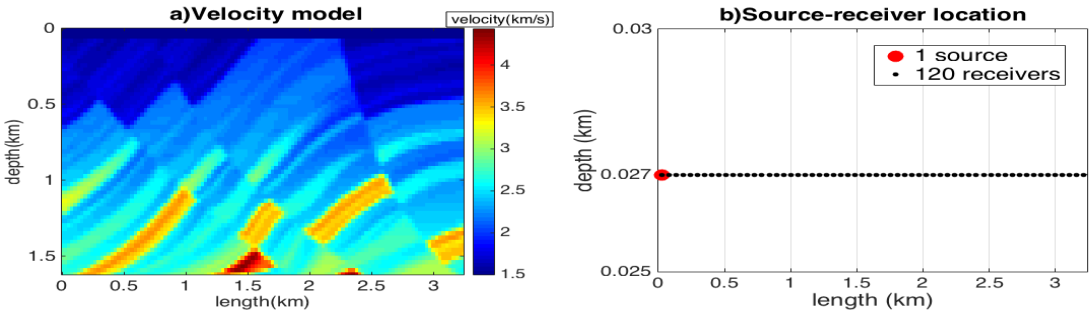


Figure 1: (a) The velocity model and (b) the source-receiver location.

length of $T = 2s$, a Ricker wavelet with $f_{max} = 30Hz$ and we set $dt = 2ms$, $dx = 27m$. We compare twelve different solutions obtained with different orders of approximation of the spatial derivatives, identical for all the grid nodes, and an implementation that optimizes the order of approximation of the spatial derivatives for a grid node as a function of the local dispersion inequality. We report in Fig. 2a the misfit values between the twelve seismograms and an "exact" seismogram computed by a numerical solution with $dx = 9$ and $p = 24$, while in Fig.2b we report the calculation time. As we can note, the optimized solution has a misfit value similar to the solution with $p = 24$, but the calculation time is similar to the solution with $p = 18$.

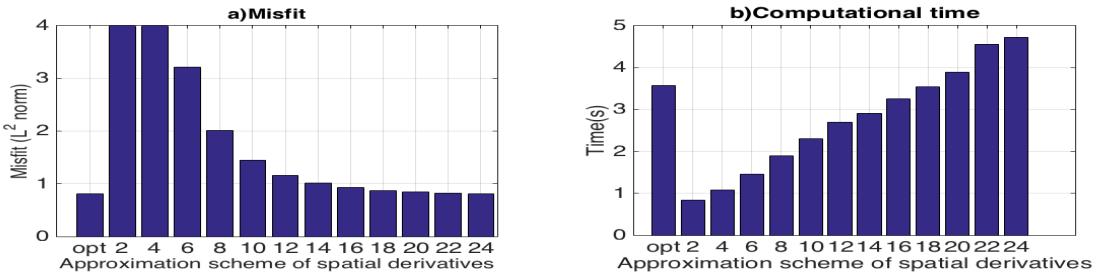


Figure 2: (a) Misfit function and (b) execution time as a function of the numerical scheme.

In conclusion our numerical scheme allows to create an adapting stiffness matrix to approximate the Laplacian operator that can be a good compromise between the simplicity of the classical finite difference method and the adaptivity of the finite element method.

References

[1] Alford, R. M., Kelly, K. R., and Boore, D. M. (1974). Accuracy of finite difference modeling of the acoustic wave equation. Geophysics , 39 (6), 834-842.

[2] Bourgeois, A., Bourget, M., Lailly, P., Ricarte, P., and Versteeg, R. (1991). Marmousi, model and data. European Association of Exploration Geophysicists.

[3] Tarantola, A. (1986). A strategy for nonlinear elastic inversion of seismic reflection data. Geophysics , 51, 1893-1903.

Analysis of a growth model and an analogue stochastic process

Serena Spina
Università degli Studi di Salerno
Via Giovanni Paolo II, 132, 84084 Fisciano (SA), Italy
sspina@unisa.it

Antonio Di Crescenzo
Università degli Studi di Salerno
Via Giovanni Paolo II, 132, 84084 Fisciano (SA), Italy
adicrescenzo@unisa.it

Constructing mathematical models of real evolutionary phenomena is relevant in many fields. It is well known that the exponential curve is a basic model for the description of growth without constrains. However, limitations of the availability of nutrients and habitat, for example, make the exponential curve not appropriate for the description of long-term growth. Alternative formulations of growth models, mainly involving regulatory effects, have been proposed in the past to take into account that the population growth slows down when the resources run out, such as the logistic model and its generalizations, power, generalized von Bertalanffy, specialized von Bertalanffy, Richards, Smith, Blumberg, hyperbolic, generic, Schnute models (see, for example [5]).

Furthermore, in various settings the constant growth rate is substituted by a time-dependent rate. When it is replaced by a decreasing exponential function we obtain the Gompertz model of population growth, whereas another choice leads to the Korf type model.

In this work we introduce a new model of population growth, which is able to describe growth phenomena sharing some characteristics of the Gompertz and Korf laws:

$$N(t) = y \exp\left\{\frac{\alpha}{\beta}\left[1-(1+t)^{-\beta}\right]\right\}, \quad t>0, \qquad N(0)=y>0, \quad \alpha,\, \beta>0.$$

In particular, it has the same initial value and same initial slope of the Gompertz law, but for large times it grows slower than the Gompertz law, as well as the Korf curve. The new model has the same carrying capacity of the other two, but it is able to capture different evolutionary dynamics. The main properties of $N(t)$ are investigated, with special attention to the correction function, the relative growth rate, the inflection point, the maximum specific growth rate, the lag time and the threshold crossing problem. A comparison to the Gompertz and Korf models is also performed. Moreover, some data analytic examples are considered in order to show that the new model can better describe some evolutionary phenomena with respect to the other ones.

However, stochastic fluctuations often are essential to describe real growth phenomena. Indeed, some growth models have been already formulated in the stochastic environment. For example, two examples of density-dependent birth-death processes whose means satisfy the logistic and Gompertz equations are given in [3], and a general theory for some non-homogeneous density-dependent birth-death processes has been developed in

[4] with special applications to stochastic logistic growth. Other families of transient birth-death processes suitable to describe population growth have been studied recently in Di Crescenzo *et al.* [1]. Moreover, diffusion stochastic processes have been proposed to take into account environmental fluctuations.

In agreement with some of the previously mentioned investigations, we construct and study two suitable stochastic processes whose means correspond to the proposed growth model: a non-homogeneous birth-death process, and a simple birth process.

In particular, we analyze the transition probabilities, the mean, the variance and the population extinction probability of the non-homogeneous birth-death process. However, we point out that even though the birth-death process considered before has conditional mean identical to the growth curve, it is not appropriate to describe a "growth behavior" in strict sense, since its sample paths can be absorbed at 0. In order to describe a pure growth phenomenon, we investigate a simple birth process mimicking the new growth model, giving attention to its transition probabilities, the mean, the variance and the first passage time problem.

Finally, our study is supported by a scrutinized analysis of the model behaviour for different choices of the involved parameters.

References

[1] Di Crescenzo, A., Giorno, V., Nobile. A.G. 2016 *Constructing transient birth–death processes by means of suitable transformations*. Appl Math Comput, 281, 152–171

[2] Di Crescenzo, A., Spina, S. 2016 *A new model of population growth*. Poster presented at the International Workshop "Stochastic Models And Related Topics", University of Salerno

[3] Parthasarathy, P.R., Krishna Kumar, B. 1991 *A birth and death process with logistic mean population*. Communications in Statistics - Theory and Methods, 20:2, 621-629, DOI: 10.1080/03610929108830519

[4] Tan, W.Y., Piantadosi, S. 1991 *A stochastic growth processes with application to stochastic logistic growth*. Statistica Sinica, 1, 527–540

[5] Tsoularis, A., Wallace, J. 2012 *Analysis of logistic growth models*. Mathematical Biosciences. 179, 21–55

Optimised prefactored compact schemes for wave propagation phenomena

Ivan Spisso
SuperComputing Application and Innovation Department, Cineca
via Magnanelli 6/3, 40033 Casalecchio di Reno, Italy
i.spisso@cineca.it

A. Rona
Department of Engineering, University of Leicester
Leicester, LE1 7RH, England
ar45@leicester.ac.uk

E. Hall
Department of Engineering, University of Leicester
Leicester, LE1 7RH, England
eh171@leicester.ac.uk

M. Bernardini
Università degli Studi di Roma "La Sapienza", Dipartimento di Meccanica e Aeronautica,
Via Eudossiana 18, 00184 Roma, Italy
matteo.bernardini@uniroma1.it

S. Pirozzoli
Università degli Studi di Roma "La Sapienza", Dipartimento di Meccanica e Aeronautica,
Via Eudossiana 18, 00184 Roma, Italy
sergio.pirozzoli@uniroma1.it

A family of space- and time-optimised prefactored compact schemes are developed that minimize the computational cost for given levels of numerical error in wave propagation phenomena,with special reference to aerodynamic sound. This work extends the approach of [2] to the class of prefactored compact high-order schemes developed by [1], in which their shorter stencil from the prefactorization leads to a simpler enforcement of numerical boundary conditions. Theoretical predictions for spatial and temporal error bounds are derived for the cost-optimized schemes and compared against benchmark schemes of current use in computational aeroacoustic applications in terms of computational cost for a given relative numerical error value. One- and two-dimensional test cases are presented to examine the effectiveness of the cost-optimized schemes for practical flow computations. An effectiveness up to about 50% higher than standard schemes is verified for the linear one-dimensional advection solver, which is a popular baseline solver kernel for computational physics problems. Substantial error reduction for a given cost is also obtained in the more complex case of a two-dimensional acoustic pulse propagation, provided the optimized schemes are made to operate close to their nominal design points. The present contribution, which is a follow-up of the work [3], provides a first verification of the predictive performance of a computational cost estimator of simple formulation,

showing that this linearly relates to the actual computational time recorded in numerical experiments on a high performance cluster. This work enables tailoring spatial and temporal coefficients of the prefactored compact finite-difference time-marching schemes to obtain aeroacoustic predictions within computational cost and numerical error bounds.

References

[1] Hixon, R., 2000 *Prefactored small-stencil compact schemes.* Journal of Computational Physics 165, 522–41.

[2] Pirozzoli, S. 2007 *Performance analysis and optimization of finite difference schemes for wave propagation problems.* Journal of Computational Physics 222, 809–831.

[3] Spisso, I. Rona, A. and Pirozzoli, S. 2014 *Development of a family of cost-optimized prefactored high-order compact schemes for low-speed aeroacoustics.* SIMAI 2014 Biannual Congress of the Società Italiana di Matematica Applicata e Industriale

Wrinkling in poked pressurized shallow shells

Matteo Taffetani
Mathematical Institute, University of Oxford
Woodstock Rd OX2 6GG, Oxford - United Kingdom
matteo.taffetani@maths.ox.ac.uk

Dominic Vella
Mathematical Institute, University of Oxford
Woodstock Rd OX2 6GG, Oxford - United Kingdom
dominic.vella@maths.ox.ac.uk

Poking a pressurized shallow shell can, depending on its geometrical properties and the loading conditions applied, lead to surprising behaviour such as wrinkling. Using both analytical approaches and finite element simulations, this work aims to investigate the behaviour of indented pressurized shells, both near- and far- from the wrinkling threshold.

We considered the equations of the plate theory modified by including the effect of a radius of curvature and we investigate the dimensionless problem that depends on a single parameter τ, related to the tension in the shell due to the inflation. With a classic linear stability analysis, we compute both the critical indentation depth δ_c at the onset of wrinkling and the wavenumber m of the wrinkles at the onset. Energy arguments reveal a novel scaling of wrinkle number with τ, highlighting the presence of an intermediate regime for pressurization that are large but not too large. The problem of the indentation of a shell is implemented in the finite element software Abaqus. Numerical results agree with the scaling predictions and show that, in the case of large pressurization, the wrinkle number increases with radial position and decreases for larger indentation depths. This spatial variation of the wrinkle wavelength λ is investigated using the recently proposed local λ law [1].

References

[1] J.D. Paulsen, E. Hohlfeld, H. Kinga, J. Huanga, Z. Qiua, T.P. Russell, N. Menon, D. Vella and B. Davidovitch, Curvature-induced stiffness and the spatial variation of wavelength in wrinkled sheets. *PNAS* 113(5):1144-1149, 2016.

Statistical Calibration Of Numerical Models With Application To ECG Models

Nicholas Tarabelloni
Politecnico di Milano
Via Bonardi 9, 20133 Milano, Italy
nicholas.tarabelloni@polimi.it

Elisa Schenone
University of Luxembourg
6 Rue Richard Coudenhove-Kalergi, 1359 Luxembourg, Luxembourg
elisa.schenone@uni.lu

Annabelle Collin
Université de Bordeaux
351, cours de la Libération - F 33 405 Talence, France
annabelle.collin@inria.fr

Francesca Ieva
Università degli Studi di Milano
via Saldini 50, 20133 Milano, Italy
francesca.ieva@unimi.it

Anna Maria Paganoni
Politecnico di Milano
Via Bonardi 9, 20133 Milano, Italy
anna.paganoni@polimi.it

Jean-Frédéric Gerbeau
Inria - Paris
2 rue Simone Iff, CS 42112, 75589 Paris Cedex 12
jean-frederic.gerbeau@inria.fr

When dealing with parametrised numerical models an interesting point is the study of possible choices of parameters yielding a response with desired features. In this case, special care must be taken in selecting an appropriate reference output to which the numerical model should be calibrated. We consider the case of a numerical model with functional response, i.e. a model whose output quantity of interest depends on a continuous variable (e.g. time or space). An example can be the case of models for human electrophysiology, where the functional output is a synthetic electrocardiogram (ECG). We also consider to have a set of real (functional) observations, which can be thought as empirical realisations of the phenomenon described by the model or as a benchmark dataset, which we want to use to calibrate the model and reproduce its important features. We propose a novel statistical method that, instead of focusing on a single representative of the dataset, performs the calibration by using the whole dataset. Due to the complex nature of infinite-dimensional data, we exploit the statistical framework of Functional

Data Analysis (FDA) and the recently proposed notion of spatial quantiles for functional data to obtain a general and flexible family of calibration problems. This method, that can be interpreted as a form of nonlinear quantile regression for functional data, yields as special case the calibration to the (spatial) median of the reference dataset, but other quantiles can be profitably specified as well. We apply this technique to the case of differential models (ODE and PDE based) for the in-silico simulation of human ECGs, and we show the results of calibration to a real dataset of physiological traces.

Inertia-like behavior in magnetization dynamics: a numerical approximation

Mouhcine Tilioua
M2I Laboratory, MAMCS Group
FST Errachidia, P. O. Box 509 Boutalamine
52000 Errachidia
Morocco
m.tilioua@fste.umi.ac.ma

We consider a mathematical model arising in micromagnetism. The model describes magnetization dynamics with inertial effetcs. We first prove global existence of weak solutions by using Faedo-Galerkin method. A semi- implicit finite difference scheme for the model is then proposed and a criterion of numerical stability is given. Some numerical experiments are conducted to show the performance of the scheme.

References

[1] J.-E. Wegrowe and M. C. Ciornei, Magnetization dynamics, gyromagnetic relation, and inertial effects, Am. J. Phys., **80** (2012), 607.

[2] E. Olive, Y. Lansac, M. Meyer, M. Hayoun and J.-E. Wegrowe, Deviation From the Landau-Lifshitz-Gilbert equation in the Inertial regime of the Magnetization, J. Appl. Phys., **117** (2015), 213904.

[3] M. Hadda and M. Tilioua, On magnetization dynamics with inertial effects, J. Engineering Mathematics, **88** (2014), 197–206.

Fluid-Structure Interaction Applied to Valve Dynamics via the Extended Finite Element Method

Stefano Zonca
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
stefano.zonca@polimi.it

Luca Formaggia
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
luca.formaggia@polimi.it

Christian Vergara
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
christian.vergara@polimi.it

In this talk, we present an eXtended Finite Element Method (XFEM) to simulate the fluid-structure interaction arising from a 3D flexible thick structure immersed in a fluid in presence of large displacements. The XFEM approach is able to treat discontinuities of the numerical solution along an interface that it is allowed to cross the elements, by enriching the approximation space with additional degrees of freedom [2]. The idea is to discretize independently the fluid and solid domains by generating two overlapped unstructured meshes and to consider the fluid-structure interface as a discontinuity for the fluid mesh. Due to the unfitted nature of the considered meshes, this method avoids the technical problems related to an Arbitrary Lagrangian-Eulerian (ALE) approach while maintaining an accurate description of the fluid-structure interface. The coupling between fluid and solid is taken into account by means of a Discontinuous Galerkin approach, which allows to weakly impose the interface conditions. The same framework was recently adopted in [1] and [3]. A possible application is the study of the interaction arising between blood and aortic valve leaflets since it is important for understanding their functional behaviour, for developing prosthetic valve devices and for post-surgery feedbacks.

References

[1] Alauzet, F., Fabrèges, B., Fernández, M. A. and Landajuela, M. 2016 *Nitsche-XFEM for the coupling of an incompressible fluid with immersed thin-walled structures.* Comput. Methods Appl. Mech. Engrg. 301, 300–335.

[2] Hansbo, A. and Hansbo, P. 2002 *An unfitted finite element method, based on Nitsche's method, for elliptic interface problems.* Comput. Methods Appl. Mech. Engrg. 191, 5537–5552.

[3] Massing, A., Larson, M. G. and Logg, A. 2013 *Efficient implementation of finite element methods on nonmatching and overlapping meshes in three dimensions*. SIAM J. Sci. Comput. 35 (1), C23–C47.

Fully stable and fully consistent nonconforming Galerkin methods

Pietro Zanotti
Università degli Studi di Milano
via Festa del Perdono, 7 20122 - Milano Italy
pietro.zanotti@unimi.it

Andreas Veeser
Università degli Studi di Milano
via Festa del Perdono, 7 20122 - Milano Italy
andreas.veeser@unimi.it

We consider symmetric and elliptic linear variational problems in a Hilbert space V. Generalizing standard conforming discretizations, we propose a nonconforming Galerkin method, which is fully stable and fully consistent. The first property guarantees that, for any load term in V', the approximating function is well-defined and bounded in the energy norm. The second one ensures that the consistency error vanishes in V. Combining full stability and full consistency, we prove that our approximation is near-best and determine the quasi-optimality constant. We apply this framework to the discretization of second- and fourth-order model problems with the Crouzeix-Raviart and Morley element respectively.

Minisymposia

Applications and Numerical Methods for Integral Equations - Part I

PROPOSERS

Alessandra Aimi
Università di Parma
Parco Area delle Scienze, 53/A 43124 - Parma Italy
alessandra.aimi@unipr.it

Mauro Diligenti
Università di Parma
Parco Area delle Scienze, 53/A 43124 - Parma Italy
mauro.diligenti@unipr.it

Silvia Falletta
Politecnico di Torino
Corso Duca degli Abruzzi, 24 10129 - Torino Italy
silvia.falletta@polito.it

Chiara Guardasoni
Università di Parma
Parco Area delle Scienze, 53/A 43124 - Parma Italy
chiara.guardasoni@unipr.it

Maria Lucia Sampoli
Università di Siena
Via Roma, 56 53100 - Siena Italy
sampoli@unisi.it

SPEAKERS

Stefano Serra Capizzano
Dept. Physics and Mathematics, Università dell'Insubria
stefano.serrac@uninsubria.it

Alessandra Sestini
Dept. Mathematics and Computer Science, Università di Firenze
alessandra.sestini@unifi.it

Alessandra Aimi
Dipartimento di Matematica e Informatica, Università di Parma
alessandra.aimi@unipr.it

Silvia Falletta
Dipartimento Scienze Matematiche, Politecnico di Torino
silvia.falletta@polito.it

Eleonora Messina
Dipartimento di Matematica e Applicazioni, Università di Napoli Federico II

eleonora.messina@unina.it

Patrick Fedeli
Dipartimento di Ingegneria Civile e Ambientale, Politecnico di Milano
patrick.fedeli@polimi.it

Integral equations and related numerical methods have reached nowadays a high level of maturity and applicability, which is documented by an enormous number of topics, e.g., acoustics, electromagnetics, elastodynamics, heat conduction, fluid mechanics, wave propagation, meteorology, space research, soil-structure interactions, geotechnical applications, geophysics, seismology, imaging and so on, and have become an outstanding example of high degree of interaction between numerical analysis, engineering and applied sciences. Despite this level of maturity, new theoretical results, numerical methods and applications seem to occur with an impressive speed. As a consequence, the purpose of this minisymposium is to present some of these significant new mathematical and computational developments, involving also issues of numerical integration, approximation theory, fast boundary element methods also coupled with finite elements or finite difference methods, and related recent applications. Theoretical and practical contributions are highly welcome.

Spectral Analysis of matrices coming from approximations of Integral Operators

Stefano Serra Capizzano
Università degli Studi dell'Insubria - Sede di Como- DISAT
via Valleggio, 11 22100 - Como Italy
Uppsala University - Information Technology Department
Box 337, SE-751 05 - Uppsala, Sweden
stefano.serrac@uninsubria.it, stefano.serra@it.uu.se

Let $k(\cdot,\cdot)$ be a continuous kernel defined on $\Omega \times \Omega$, Ω bounded subset of $\mathbb{R}^d$, $d \geq 1$, and let us consider the integral operator $\tilde{K}$ from $\mathcal{C}(\Omega)$ into $\mathcal{C}(\Omega)$ ($\mathcal{C}(\Omega)$ set of continuous functions on Ω) defined as the map

$$f(x) \to l(x) = \int_\Omega k(x,y) f(y)\,\mathrm{d}y, \quad x \in \Omega.$$

$\tilde{K}$ is a compact operator and therefore its spectrum forms a bounded sequence having zero as unique accumulation point. Here we first consider in detail the approximation of $\tilde{K}$ by using rectangle formula in the case where $\Omega = [0,1]$ and the step is $h = 1/n$. The related linear application can be represented as a matrix A_n of size n. In accordance with the compact character of the continuous operator, we prove that $\{A_n\} \sim_\sigma 0$ and $\{A_n\} \sim_\lambda 0$, i.e., the considered sequence has singular values and eigenvalues clustered at zero. Moreover the cluster is strong in perfect analogy with the compactness of $\tilde{K}$. Several generalizations are sketched, with special attention to the general case of pure sampling sequences and to the case of boundary element approximations of partial differential equations. Few examples and numerical experiments are critically discussed, including the use of GMRES and preconditioned GMRES for large linear systems coming from the numerical approximation of integral equations of the form

$$((I - \tilde{K})f(t))(x) = g(x), \quad x \in \Omega, \tag{1}$$

with $(\tilde{K}f(t))(x) = \int_\Omega k(x,y)f(y)\,\mathrm{d}y$ and datum $g(x)$.

References

[1] Al-Fhaid A. S., Serra-Capizzano S., Sesana D., Ullah M. Z. *Singular-value (and eigenvalue) distribution and Krylov preconditioning of sequences of sampling matrices approximating integral operators.* Numer. Linear Algebra Appl. 21 (2014) 722–743.

[2] Salinelli E., Serra-Capizzano S., Sesana D. *Eigenvalue-eigenvector structure of Schoenmakers–Coffey matrices via Toeplitz technology and applications.* Linear Algebra Appl. 491 (2016) 138–160.

Development of a basis–oriented assembly strategy suited for Isogemetric Galerkin BEMs

Alessandra Sestini
Università degli Studi di Firenze
viale Morgagni 67/a, Firenze Italy
alessandra.sestini@unifi.it

Alessandra Aimi
Università di Parma
Parco Area delle Scienze, 53/A, Parma Italy
alessandra.aimi@unipr.it

Francesco Calabrò
Università di Cassino e del Lazio Meridionale
Via G. De Biasi 43, Cassino Italy
calabro@unicas.it

Mauro Diligenti
Università di Parma
Parco Area delle Scienze, 53/A, Parma Italy
mauro.diligenti@unipr.it

Mara Lucia Sampoli
Università di Siena
Via Roma, 56, Siena Italy
sampoli@unisi.it

For several elliptic, parabolic and hyperbolic interior and exterior problems, the fundamental solution of the related differential operator is known and this makes possible their reformulation into boundary integral equations. Boundary Element Methods (BEMs) combined with collocation or Galerkin techniques can then be applied to approximate the related solution with the remarkable advantage that the discretization process is applied on a domain with dimension reduced by one. Even if the first BEM implementations required a preliminary tiling of the boundary, already in the nineties a more robust formulation, called *curvilinear* BEMs, was introduced to avoid such drawback. Actually, the linear space used for the discretization by the curvilinear approach is obtained by lifting to the boundary geometry a basis directly defined in the whole parametric boundary domain. Thus we can say that the isogeometric formulation of BEMs (IGA–BEMs) recently introduced in the literature (see e.g. [4] and references therein) goes further in this direction because, considering that in the engineering context usually the boundary is assigned in B–spline form by standard CAD tools, IGA–BEMs use such functions also to generate the discretization space. Traditionally, as well as in the context of finite element methods, the Lagrangian basis of a certain degree d was adopted which is nothing but a special basis of the space of d–degree splines with just C^0 smoothness at the knots.

Thus the IGA–BEMs are also much more flexible because the B–spline basis adopted for the discretization can be any refinement of the B–spline basis used by the CAD tools to define the boundary (for example multiple knots can be used in order to reduce the regularity required at some point). As a consequence of a discretization based on more regular spaces and in particular on B-splines, it seems almost a necessary step to switch from the traditional *element–by–element* assembly phase to a *basis–oriented* one, in order to speed-up the generation of the final linear system of equations.
Focusing on a symmetric Galerkin BEM (SGBEM), in this talk we will first of all show the performances of its isogeometric formulation [2] which has been checked by using a standard assembly phase. A key point of the preliminary code used for the experiments is its relying on highly accurate quadrature formulas applied on each boundary element to deal with the involved singular kernels [1]. Now, we are moving to a more efficient basis-oriented assembly phase, based on the development of new quadrature schemes, specific for integrals involving singular kernels, B-splines and boundary geometry. These integrals are split in the sum of a regular contribution, numerically evaluated using formulas given in [3] and a singular one treated by quadrature rules employing the so-called B-spline moments evaluated analytically. Preliminary results related to this new quadrature strategy will be also shown in the talk.

References

[1] A. Aimi, M. Diligenti and G. Monegato 1999 *Numerical integration schemes for the BEM solution of hypersingular integral equations*. Int. J. Numer. Meth. Engng. 45, 1807–1830.

[2] A. Aimi, M. Diligenti, M. L. Sampoli and A. Sestini 2016 *Isogeometric Analysis and Symmetric Galerkin BEM: a 2D numerical study*. Applied Mathematics of Computation 272, 173–186.

[3] F. Calabrò, C. Manni and F. Pitolli 2015 *Computation of quadrature rules for integration with respect to refinable functions on assigned nodes*. Appl. Numer. Math 90, 168–189.

[4] R. Simpson, M. Scott, M. Taus, D. Thomas and H. Lian 2014 *Acoustic isogeometric boundary element analysis*. Comput. Methods Appl. Mech. Engrg., 269, 265–290.

Energetic BEM for the numerical analysis of damped wave propagation exterior problems

Alessandra Aimi
Università degli Studi di Parma
viale Parco Area delle Scienze, 53/A 43124 - Parma Italy
alessandra.aimi@unipr.it

Mauro Diligenti
Università degli Studi di Parma
viale Parco Area delle Scienze, 53/A 43124 - Parma Italy
mauro.diligenti@unipr.it

Chiara Guardasoni
Università degli Studi di Parma
viale Parco Area delle Scienze, 53/A 43124 - Parma Italy
chiara.guardasoni@unipr.it

The analysis of damping phenomena that occur in many physics and engineering problems, such as fluid dynamics, kinetic theory and semiconductors, is of particular interest. In waves propagation, the dissipation is generated by the interaction between the waves and the propagation medium and it can be also closely related to the dispersion. For the numerical solution of these types of problems, one needs accurate and stable approximations even on large time intervals.
In this context, time-dependent problems modeled by linear hyperbolic partial differential equations (PDEs) can be reformulated, knowing the fundamental solution of the partial differential operator at hand, in terms of boundary integral equations (BIEs) on the usually bounded surface of the domain and solved via boundary element methods (BEMs) [6].
Here, starting from a recently developed energetic space-time weak formulation, applied in particular to the BIEs related to classical wave propagation problems exterior to obstacles [1, 2], and using the so-called Energetic BEM as discretization technique, we consider an extension for the damped wave equation in 2D space dimension, based on successful simulations related to the 1D case [3, 4, 5].
Several numerical results, for different values of viscous and material damping coefficients, will be presented and discussed, showing high accuracy and large time stability of the obtained approximate solutions, both on the obstacles and around them.

References

[1] Aimi, A., Diligenti, M., Guardasoni, C., Mazzieri, I. and Panizzi, S. 2009, *An energy approach to space–-time Galerkin BEM for wave propagation problems*. International Journal for Numerical Methods in Engineering. 80, 1196–1240.

[2] Aimi, A., Diligenti, M. and Panizzi 2010, S. *Energetic Galerkin BEM for wave propagation Neumann exterior problems*. CMES, 58(2), 185–219.

[3] Aimi, A. and Panizzi 2014, *BEM-FEM Coupling for the 1D Klein–-Gordon Equation*. Numer. Methods Partial Differential Eq., 30, 2042–2082.

[4] Aimi, A., Diligenti, M. and Guardasoni, C. 2015, *Comparison between numerical methods applied to damped wave equation*. Journal of Integral Equations and Applications, submitted.

[5] Aimi, A., Diligenti, M. and Guardasoni, C. 2016, *Energetic BEM-FEM coupling for the numerical solution of the damped wave equation*. International Journal for Numerical Methods in Engineering, submitted.

[6] Vick, B. and West, R.L. 1997, *Analysis of Damped Waves Using the Boundary Element Method*. Transaction on Modelling and Simulation, 15, 265–278.

On the discretization of a space-time boundary integral equation for the numerical solution of 3D time dependent scattering problems

Silvia Falletta
Dip. Scienze Matematiche - Politecnico di Torino
Corso Duca degli Abruzzi, 24 10129 - Torino Italy
silvia.falletta@polito.it

Giovanni Monegato
Dip. Scienze Matematiche - Politecnico di Torino
Corso Duca degli Abruzzi, 24 10129 - Torino Italy
giovanni.monegato@polito.it

Letizia Scuderi
Dip. Scienze Matematiche - Politecnico di Torino
Corso Duca degli Abruzzi, 24 10129 - Torino Italy
letizia.scuderi@polito.it

In the last decades, space-time Boundary Integral Equations (BIEs) have been successfully applied to wave propagation problems defined in the exterior of a bounded domain. Most of them, however, are for homogeneous problems with trivial initial data. Furthermore, the BIE is generally used to determine the problem solution at chosen points of the domain. Only in the last couple of years (see [1], [3],[2]), a BIE for the classical wave equation has been used to define a Non Reflecting Boundary Condition (NRBC) on a chosen artificial boundary, surrounding the computational domain. Its discretization is then coupled with that of the domain of interest by means of finite elements or finite differences. In the case of the classical 3D non homogeneous wave equation, the problem we consider is the following:

$$\begin{cases} \frac{1}{c^2}u^e_{tt}(\mathbf{x},t) - \Delta u^e(\mathbf{x},t) = f(\mathbf{x},t) & \text{in } \Omega^e \times (0,T) \\ u(\mathbf{x},t) = g(\mathbf{x},t) & \text{in } \Gamma \times (0,T) \\ u^e(\mathbf{x},0) = u_0(\mathbf{x}) & \text{in } \Omega^e \\ u^e_t(\mathbf{x},0) = v_0(\mathbf{x}) & \text{in } \Omega^e. \end{cases} \tag{1}$$

where $\Omega^e = \mathbb{R}^3 \setminus \overline{\Omega^i}$, Ω^i being a bounded open domain, having a smooth boundary Γ, or the union $\cup_{k=1}^{\kappa}\Omega^i_k$ of well separated domains of this type. The BIE we consider for the numerical solution of (1) is the following single layer-double layer one (see [3]):

$$\frac{1}{2}u(\mathbf{x},t) = \int_0^t \int_\Gamma G(\mathbf{x}-\mathbf{y},t-\tau)\partial_{\mathbf{n}}u(\mathbf{y},\tau)d\Gamma_{\mathbf{y}}d\tau - \int_0^t \int_\Gamma \partial_{\mathbf{n}}G(\mathbf{x}-\mathbf{y},t-\tau)u(\mathbf{y},\tau)d\Gamma_{\mathbf{y}}d\tau + I_{u_0}(\mathbf{x},t) + I_{v_0}(\mathbf{x},t) + I_f(\mathbf{x},t) \quad \mathbf{x}\in\Gamma, \tag{2}$$

where $\partial_{\mathbf{n}} = \partial\mathbf{n}_{\mathbf{y}}$ denotes the outward unit normal derivative on the boundary Γ, for the problem defined in Ω^e, and I_{u_0}, I_{v_0}, I_f are the "volume" integrals generated by the non

homogeneous initial conditions and the non trivial source, respectively. Very recently, in [3] (see also [2]), for the solution of (1), we have proposed to use (2) also as a global Non Reflecting Boundary Condition, to be imposed on a chosen artificial boundary $\mathcal{B}$ delimiting the domain of interest Ω. This NRBC is interpreted as a relationship that the problem solution and its normal derivative must satisfy on $\mathcal{B}$, to avoid spurious reflections. It is of exact type, and it holds for a (smooth) surface of arbitrary shape; therefore, it can be used also in situations of multiple scattering, and even in more general ones. Moreover, it allows the problem to have non trivial data, whose (local) supports do not have necessarily to be included in the Ω domain, as it is usually done, in particular when they are away from the domain of interest. In such a case, the proposed NRBC naturally includes the effects of these data and it is automatically transparent for outgoing waves as well as for incoming ones.
For the discretization of the BIE (2), or of the corresponding NRBC, namely for the approximation of the single and double layer operators, we have proposed a numerical scheme which is based on a second order Lubich discrete convolution quadrature formula (see [6]), for the discretization of the time integral, coupled with a classical collocation method in space. Its computational complexity is of order $N \log N$, being N the total number of time steps performed, while that of the global (space-time) discretization is of order $M^2 N \log N$, where M is the number of collocation points chosen on the domain surface. The required working storage is $M^2 N$. We recall that, when the discretization of the bounded domain Ω (where we apply the chosen finite element scheme) is refined, and the time step-size is simultaneously reduced, the accuracy of the NRBC discretization increases.
In all the papers where the above approach has been applied, the wave propagation velocity has been taken equal to 1, and also the dimension of the physical domains is of order 1. Furthermore, the final computational time instant T is generally not large, let us say, from 1 up to about 50. Of course, by properly scaling the variables, a problem of type (1) can always be reduced to this form. For example, in the case of velocity c and domain diameter d, it is sufficient to set $\mathbf{x} = d\overline{\mathbf{x}}$ and $t = \frac{d}{c}\overline{t}$. This scaling, however, changes also the original time interval of integration $(0, T]$ into $(0, \overline{T}]$, with $\overline{T} = cT/d$. And in several applications, T is not small. This is the case, for example, of sources f far away from the domain Ω^i, or of multiple scattering - multiple sources problems, or of scattering from non convex domains having cavities; that is, wave propagation problems having a long transient phase. Thus, in these cases, $\overline{T}$ turns out to be much larger that 50.
In particular, we consider 3D wave propagation problems in unbounded domains, such as those of acoustic waves in non viscous fluids, of seismic waves in (infinite) homogeneous isotropic materials, or of electromagnetic waves, where the propagation velocity c is much higher than 1. For example, for the acoustic waves in air and water we have $c \approx 343\, m/s$ and $c \approx 1500\, m/s$, respectively, while for seismic P waves in linear solids we may have $c \approx 6000\, m/s$ or higher; for the electromagnetic waves in vacuum we have $c \approx 3E{+}08\, m/s$. We allow waves generated by sources, that can be located far away from the obstacles. Finally, we assume that the order of magnitude of the obstacles is much smaller than that of the wave velocity, and that the problem transients are not excessively short.
We show that for such problems, the computational cost and storage required by the numerical approach mentioned above can be significantly reduced by taking into account a property concerning the behavior of the coefficients of the (time) discrete convolution quadrature, that till now has been ignored. This allows to replace, in the above mentioned computational cost and working storage, the $N \log N$ and N factors by a significantly

small integer N_0.
We note that in some papers (see [5], [4]), to reduce the method computational cost storage, some sparse approximations of the matrices generated by the chosen Lubich discrete convolution have been proposed and examined. However, these do not apply to the problems we are considering. Instead, they apply to a complementary case, where velocity and obstacle have similar orders of magnitude, and the time interval of integration is not large.
To justify the above mentioned reduction, we derive some bounds for the coefficients of the discrete convolution quadrature, when the wave propagation velocity is much higher than the obstacle dimensions. These bounds show how computational cost and work storage can be significantly reduced. Then, we apply the proposed numerical approach to several acoustic problems; these include cases where the BIE plays the role of a NRBC and multiple scattering - multiple source examples.

References

[1] Aimi A., Diligenti M., Frangi A., Guardasoni, C., Energetic BEM-FEM coupling for wave propagation in 3D multidomains, Internat. J. Numer. Methods Engrg. 97 (2014), 377-394.

[2] Banjai L., Lubich Ch., Sayas F.-J., Stable numerical coupling of exterior and interior problems for the wave equation. Numer. Math. 129 (2015) 611-646.

[3] Falletta S., Monegato G., Exact non-reflecting boundary condition for 3D time-dependent multiple scattering-multiple source problems. Wave Motion 58 (2015), 281-302.

[4] Falletta S., Sauter S., The panel-clustering method for the wave equation in two spatial dimensions, J. Comput. Phys. 305 (2016) 217-243.

[5] Hackbusch W., Kress W., Sauter S., Sparse convolution quadrature for time domain boundary integral formulations of the wave equation, IMA J. Numer. Anal. 29(1) (2009) 158-179.

[6] Lubich Ch., Convolution quadrature and discretized operational calculus. I, Num. Math. 52 (1988) 129-145.

Stability of numerical solutions to Abel-Volterra integral equations of the second kind

Eleonora Messina
Università degli Studi di Napoli "Federico II"
via Cintia, 80126 - Napoli Italy
eleonora.messina@unina.it

Roberto Garrappa
Università degli Studi di Bari
via E.Orabona 4, 70125 - Bari Italy
roberto.garrappa@uniba.it

Antonia Vecchio
C.N.R. National Research Council of Italy
via P. Castellino 111, 80131 - Napoli Italy
antonia.vecchio@cnr.it

We analyse the numerical approximation, by product integration rules, of Abel-Volterra integral equations of the second kind over long-time intervals. We study the stability with respect to a new class of non-parametric test equations and we investigate how the analytical and the numerical solution respond to certain perturbations in the kernel.
This analysis extends to weakly singular equations the results obtained for regular kernels in continuous [1] and discrete [2] equations.

References

[1] de Hoog, F. R.; Anderssen, R. S. 2012 *Kernel perturbations for a class of second-kind convolution Volterra equations with non-negative kernels.* Appl. Math. Lett. 25 , no. 9, 1222 -1225.

[2] Messina, E.; Vecchio, A. 2016 *A sufficient condition for the stability of direct quadrature methods for Volterra integral equations.* Submitted.

Integral equations for free-molecule flow in MEMS microstructures: recent advancements

Patrick Fedeli
DICA Department, Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
patrick.fedeli@polimi.it

Attilio Frangi
DICA Department, Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
attilio.frangi@polimi.it

Gabriele Gattere
AMS Division, STMicroelectronics
Via Tolomeo, 1 20010 - Cornaredo Italy
gabriele.gattere@st.com

This work proposes an innovative simulation tool for the prediction of gas damping occurring in MEMS working in near vacuum at frequencies just above the audio band (i.e. around 20kHz). Recent improvements in the implementation based on multi-core parallelism and concepts of computer graphics allow to address almost full-scale realistic MEMS. Three different families of test devices (an example in Figure 1) have been designed, fabricated, tested and simulated, in order to confirm the ability of the numerical model. The groups represent standard building blocks of MEMS working in these conditions. Tests have been operated both at variable pressures in a vacuum chamber and in the closed package and demonstrate an accuracy in the order of 15%.

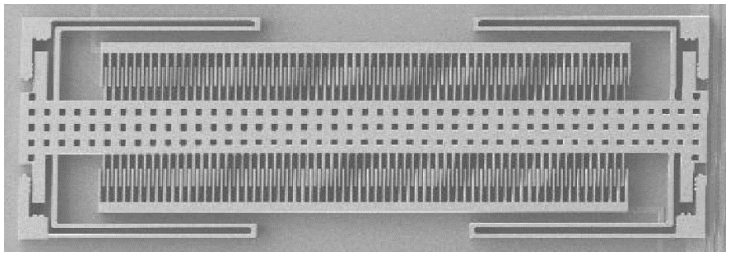


Figure 1: SEM overview of a comb-finger (CF) structure

Numerical model The deterministic model implemented for the simulation, proposed in [4, 3], is an application of the collisionless Boltzmann equation [1, 2] which rests on the following assumptions: i) the mean free-molecule path is much larger than the typical dimension d of the flow (i.e. Kn$\gg$1); ii) molecules and solid surfaces interact according the diffuse-reflection model which basically states that molecules are re-emitted by the walls according to the wall equilibrium Maxwellian; iii) perturbations are small so that quadratic terms in the expansion of variables can be neglected. Moreover, if frequency f

of perturbations is slow with respect to thermal velocity, i.e. $d \times f/\sqrt{2\mathcal{R}T_0} \ll 1$ ($\mathcal{R}$ is the universal gas constant divided by the molar mass and T_0 is the package temperature), the formulation can be further simplified leading to the model discussed herein. Let $J(\mathbf{x},t)$ denote the linear term in the expansion of the flux of incoming molecules at point $\mathbf{x}$ of the MEMS surface. This scalar unknown is governed by the following "quasi-static" integral equation:

$$\begin{aligned} J(\mathbf{x},t) = & \sqrt{\pi}\tilde{g}_n(\mathbf{x},t) - \\ & \frac{1}{\pi}\int_{S^+} J(\mathbf{y},t)\big(\mathbf{r}\cdot\mathbf{n}(\mathbf{x})\big)\big(\mathbf{r}\cdot\mathbf{n}(\mathbf{y})\big)\frac{1}{r^4}\mathrm{d}S + \\ & \frac{3}{2}\frac{1}{\sqrt{\pi}}\int_{S^+}\big(\mathbf{r}\cdot\tilde{\mathbf{g}}(\mathbf{y},t)\big)\big(\mathbf{r}\cdot\mathbf{n}(\mathbf{x})\big)\big(\mathbf{r}\cdot\mathbf{n}(\mathbf{y})\big)\frac{1}{r^5}\mathrm{d}S \end{aligned} \tag{1}$$

where $r = \|\mathbf{y}-\mathbf{x}\|$; $\mathbf{n}$ is the outward normal to the surface; S^+ denotes the portion of surface visible from $\mathbf{x}$; $\tilde{\mathbf{g}}(\mathbf{y},t) = \mathbf{g}(\mathbf{y},t)/\sqrt{2\mathcal{R}T_0}$ is the normalised velocity of surfaces, $\tilde{g}_n = \tilde{\mathbf{g}}\cdot\mathbf{n}$ being its projection along $\mathbf{n}$. A posteriori a second integral equation provides the distribution of perturbation forces $\mathbf{t}$ on the structure:

$$\begin{aligned} -\frac{\mathbf{t}(\mathbf{x},t)}{\rho_0 2\mathcal{R}T_0} = & \frac{1}{4}J(\mathbf{x},t)\mathbf{n}(\mathbf{x}) + \frac{1}{\sqrt{\pi}}\tilde{g}_n(\mathbf{x},t)\mathbf{n}(\mathbf{x}) + \frac{1}{2\sqrt{\pi}}\tilde{\mathbf{g}}_t(\mathbf{x},t) - \\ & \frac{3}{8\pi}\int_{S^+}\mathbf{r}\Big(\mathbf{r}\cdot\mathbf{n}(\mathbf{x})\Big)\Big(\mathbf{r}\cdot\mathbf{n}(\mathbf{y})\Big)\frac{1}{r^5}J(\mathbf{y},t)\mathrm{d}S + \\ & \frac{2}{\pi^{3/2}}\int_{S^+}\mathbf{r}\Big(\mathbf{r}\cdot\tilde{\mathbf{g}}(\mathbf{y},t)\Big)\Big(\mathbf{r}\cdot\mathbf{n}(\mathbf{x})\Big)\Big(\mathbf{r}\cdot\mathbf{n}(\mathbf{y})\Big)\frac{1}{r^6}\mathrm{d}S \end{aligned} \tag{2}$$

where $\tilde{\mathbf{g}}_t = \tilde{\mathbf{g}} - \tilde{g}_n\mathbf{n}$. Apart from some special case where an analytical expression for $\mathbf{t}$ is available, the numerical solution of eqs.(1)-(2) is mandatory. A large-scale parallel implementation of the two integral equations, based on OpenMP architecture, allows to simulate realistic MEMS structures. Geometrically, surfaces are represented as the

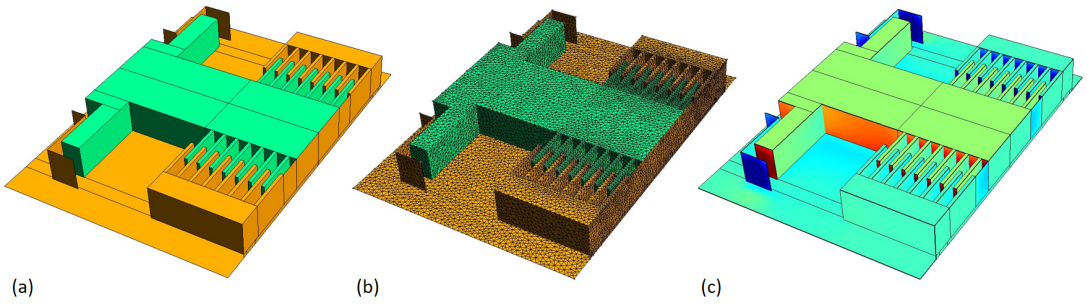


Figure 2: Example of geometric model for a portion of CF structure (a); mesh with 62526 elements (b) and force per unit surface in the direction of vibration (c)

collection of non-overlapping "large" planar quadrangles (see Figure 2-a with an example of geometric model for a portion of CF structure). This choice, which greatly simplifies testing the visibility condition, is not a severe limitation since due to technological constraints the vast majority of MEMS is composed by piecewise planar surfaces. Next, each quadrangle is meshed with triangular elements with the required degree of refinement (Figure 2-b). In the present implementation J is modeled as piecewise constant over each triangle and is computed by eq.(1) using a GMRS (Generalized minimal residual method) solver. The output of the analysis is the force $\mathbf{t}$ exerted on the surfaces along any direction

(Figure 2-c). The visibility is tested only between centers of mass of elements and the integral terms in eqs.(1)-(2) are computed using a numerical approach over Gauss points for elements far by $\mathbf{x}$ while analytically for triangles close together (see the **Appendix**). The force obtained by the simulation tool can be later post-processed as follows. The displacement $\mathbf{s}$ of the deformable MEMS is assumed to be proportional to a given vector shape function: $\mathbf{s}(\mathbf{y},t) = \boldsymbol{\psi}(\mathbf{y})q(t)$. Hence one has that $\mathbf{t}(\mathbf{x},t) = \mathbf{f}(\mathbf{x})\dot{q}(t)$, where $\mathbf{f}(\mathbf{x})$ is given by eq.(2) replacing $\mathbf{g}$ with $\boldsymbol{\psi}$. The equivalent damping term in the 1D reduced order model finally becomes:

$$\int_S \mathbf{t}(\mathbf{x},t)\boldsymbol{\psi}(\mathbf{x})\mathrm{d}S = \Big(\int_S \mathbf{f}(\mathbf{x})\boldsymbol{\psi}(\mathbf{x})\mathrm{d}S\Big)\dot{q} = B\dot{q}$$

where the integral is extended over the whole surface of the MEMS. The constant B can be conveniently expressed as

$$B = \tilde{B}\rho_0\sqrt{2\mathcal{R}T_0} = \tilde{B}p_0\sqrt{2/(\mathcal{R}T_0)} \tag{3}$$

where $\tilde{B}$ is a coefficient with the dimensions of a surface which depends only on the problem geometry.

Experiment and validation The reliability of the modeling technique which estimates dissipation was obtained through the comparison between experimental measurement and numerical computation of the quality factor Q [5]. Some of the results are collected in

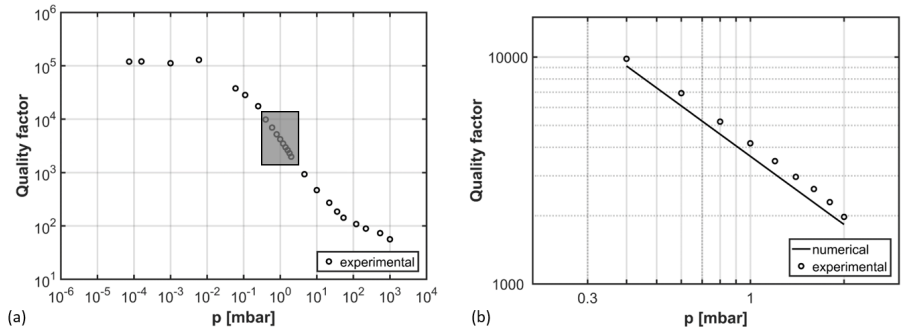


Figure 3: CF device 13: Quality factor in the whole pressure range (a); zoom in the linear region (b)

Figures 3. The former plots the quality factor in the whole pressure range for a selected CF device. A zoom of the pressure range of interest (i.e. around 1 mbar) with the comparison between simulations and experiments is plotted in the second Figure. The relative error between the two sets of data is always less than 15%.

Appendix For a given element E with center of mass $\mathbf{y}$, the generalised pyramid is defined by the connections between a source point $\mathbf{x}$ and the nodes of E. Moreover each edge e of the element and the source point $\mathbf{x}$ define a triangle of normal N_i and angle at vertex $\mathbf{x}$ equal to $\Delta\alpha$ (see Figure 4). The first integral term of eq.(1) for a given element E:

$$\int_E \big(\mathbf{r}\cdot\mathbf{n}(\mathbf{x})\big)\big(\mathbf{r}\cdot\mathbf{n}(\mathbf{y})\big)\frac{1}{r^4}\mathrm{d}S_y = n_i(\mathbf{x})\int_E \frac{r_i r_k}{r^4}n_k\mathrm{d}S_y \tag{4}$$

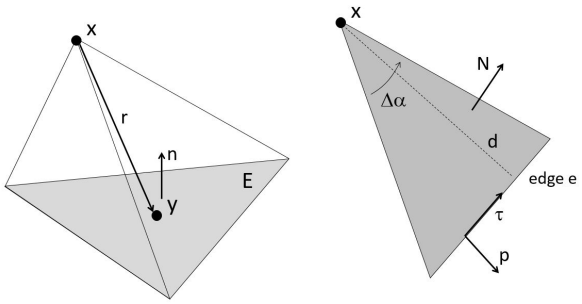


Figure 4: Generalised pyramid

$$\int_E \frac{r_i r_k}{r^4} n_k \mathrm{d}S_y = \frac{1}{2} \sum_e \Delta\alpha N_i$$

which is known as Lambert formula. The second integral term of eq.(1), which is equal to the first of eq.(2), for a given element E and a constant $\tilde{\mathbf{g}}$:

$$\int_E \big(\mathbf{r}\cdot\tilde{\mathbf{g}}\big)\big(\mathbf{r}\cdot\mathbf{n}(\mathbf{x})\big)\big(\mathbf{r}\cdot\mathbf{n}(\mathbf{y})\big)\frac{1}{r^5}\mathrm{d}S_y = \tilde{g}_i n_j(\mathbf{x}) \int_E \frac{r_i r_j r_k}{r^5} n_k \mathrm{d}S_y \tag{5}$$

$$3\int_E \frac{r_i r_j r_k}{r^5} n_k \mathrm{d}S_y = \sum_e dN_j \int_e \frac{r_i}{r^3}\,\mathrm{d}s - \delta_{ij}\Omega$$

where Ω is the solid angle at the vertex $\mathbf{x}$ of the generalised pyramid. The integral term in the second of eqs.(5) can be easily evaluated analytically. Finally, the second integral term of eq.(2) for a given element E and a constant $\tilde{\mathbf{g}}$:

$$\int_E \mathbf{r}\Big(\mathbf{r}\cdot\tilde{\mathbf{g}}\Big)\Big(\mathbf{r}\cdot\mathbf{n}(\mathbf{x})\Big)\Big(\mathbf{r}\cdot\mathbf{n}(\mathbf{y})\Big)\frac{1}{r^6}\mathrm{d}S = \tilde{g}_i n_j(\mathbf{x})\mathbf{e}_m \int_E \frac{r_i r_j r_k r_m}{r^6} n_k \mathrm{d}S_y \tag{6}$$

$$8\int_E \frac{r_i r_j r_k r_m}{r^6} n_k \mathrm{d}S_y = \sum_e \left[\Delta\alpha(N_j\delta_{im} + N_i\delta_{jm}) + 2N_m d\int_e \frac{r_i r_j}{r^4}\mathrm{d}s\right]$$

where the integral term in the second of eqs.(6) can be integrated using Lambert formula.

References

[1] Cercignani, C. 1988 *The Boltzmann equation and its applications*. Springer.

[2] Chapman, S. and Cowling, T.G. 1960 *The mathematical theory of non-uniform gases*. Cambridge University Press.

[3] Frangi, A. 2009 *BEM technique for free-molecule flows in high frequency MEMS resonators*. Engineering Analysis with Boundary Elements, 33, 493–498.

[4] Frangi, A. Ghisi, A. and Coronato, L. 2009 *On a deterministic approach for the evaluation of gas damping in inertial MEMS in the free-molecule regime*. Sensor & Actuators, A 149, 21–28.

[5] Laghi, G. Frangi, A. Fedeli, P. Gattere, G. and Langfelder, G. 2016 *Comprehensive modeling and experimental verification of air damping coefficients in MEMS of complex geometry*. Proc. MEMS 2016, Shanghai, China, pp. 958-961.

Applications and Numerical Methods for Integral Equations - Part II

PROPOSERS

Alessandra Aimi
Università di Parma
Parco Area delle Scienze, 53/A 43124 - Parma Italy
alessandra.aimi@unipr.it

Mauro Diligenti
Università di Parma
Parco Area delle Scienze, 53/A 43124 - Parma Italy
mauro.diligenti@unipr.it

Silvia Falletta
Politecnico di Torino
Corso Duca degli Abruzzi, 24 10129 - Torino Italy
silvia.falletta@polito.it

Chiara Guardasoni
Università di Parma
Parco Area delle Scienze, 53/A 43124 - Parma Italy
chiara.guardasoni@unipr.it

Maria Lucia Sampoli
Università di Siena
Via Roma, 56 53100 - Siena Italy
sampoli@unisi.it

SPEAKERS

Silvia Bertoluzza
CNR-IMATI, Pavia
silvia.bertoluzza@imati.cnr.it

Elena Loli Piccolomini
Dipartimento di Matematica Università di Bologna
elena.loli@unibo.it

Concetta Laurita
Dipartimento di Matematica, Informatica ed Economia, Università della Basilicata
concetta.laurita@unibas.it

Incoronata Notarangelo
Dipartimento di Matematica, Informatica ed Economia, Università della Basilicata
incoronata.notarangelo@unibas.it

Luisa Fermo
Dipartimento di Matematica e Informatica Università di Cagliari

fermo@unica.it

Integral equations and related numerical methods have reached nowadays a high level of maturity and applicability, which is documented by an enormous number of topics, e.g., acoustics, electromagnetics, elastodynamics, heat conduction, fluid mechanics, wave propagation, meteorology, space research, soil-structure interactions, geotechnical applications, geophysics, seismology, imaging and so on, and have become an outstanding example of high degree of interaction between numerical analysis, engineering and applied sciences. Despite this level of maturity, new theoretical results, numerical methods and applications seem to occur with an impressive speed. As a consequence, the purpose of this minisymposium is to present some of these significant new mathematical and computational developments, involving also issues of numerical integration, approximation theory, fast boundary element methods also coupled with finite elements or finite difference methods, and related recent applications. Theoretical and practical contributions are highly welcome.

A non conforming FEM-BEM coupling for wave propagation in unbounded domains

Silvia Bertoluzza
CNR - IMATI "E. Magenes"
via Ferrata 1, 2700 - Pavia Italy
silvia.bertoluzza@imati.cnr.it

Silvia Falletta
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
silvia.falletta@polito.it

Giovanni Monegato
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
giovanni.monegato@polito.it

We consider the scattering of a wave by an obstacle of $\mathbb{R}^2$, having a sufficiently smooth boundary Γ. In particular, we solve the time-dependent wave equation in the finite computational domain Ω, bounded internally by Γ and externally by an artificial boundary $\mathcal{B}$ where we impose an exact Non Reflecting (transparent) Boundary Condition (NRBC) (see [1]). The NRBC is defined through a space-time Boundary Integral Equation (BIE), which defines a relationship between the solution of the differential problem and its normal derivative on the artificial boundary $\mathcal{B}$. We discretize the BIE on $\mathcal{B}$ by combining a second order (in time) BDF convolution quadrature and a Galerkin (or a collocation) method in space. Such a discretization is then coupled with an unconditionally stable ODE time integrator and a FEM in space.

In previous works, we have tested the robustness of the proposed NRBC discretization, and its higher accuracy with respect to that of the associated FEM. Such properties justify a decoupling of the NRBC grid from that of the FEM. In particular, the discretization of the transparent condition can be constructed on a grid defined on $\mathcal{B}$ which is coarser than the one inherited by the triangulation of Ω. In this context, we propose a non conforming coupling of the FEM-BEM scheme, by using a mortar technique. The method consists in decomposing the FEM-BEM interface into two disjoint sides and in replacing the strong point-wise continuity condition of the traces of the solution on $\mathcal{B}$ by a weak one, by imposing that the jump of the traces is orthogonal to a suitable multiplier space. Such an approach allows to reduce the computational cost of the NRBC and to couple discretizations of different type. We will present numerical results obtained for problems of waves scattered by fixed and rotating obstacles, non trivial data, and sources far away from the computational domain Ω.

References

[1] S. Falletta, G. Monegato, An exact non reflecting boundary condition for 2D time-dependent wave equation problems. Wave Motion 51 (2014), no. 1, 168–192.

Regularization Methods for Image Reconstruction in Computed Tomography

Elena Loli Piccolomini
Università degli Studi di Bologna
Piazza di Porta San Donato,5 40127 - Bologna Italy
elena.loli@unibo.it

Digital Breast Tomosynthesis (DBT) is a 3D emerging technique for the diagnosis of breast tumors that has some advantages over the traditional 2D mammography suffering from the fact that the lesions can be hidden by overlaying tissues in the plane representation of a 3D object. In DBT the breast volume is reconstructed in a stack of 2D slices and the structure is resolved in space, reducing the impact of the overlapping tissues on the tumor and making easier the tumor detection by the radiologist. In DBT, usually 10-25 projections along a range of up to 40-45 degrees are obtained and from these projections a pseudo-3D representation of the object is reconstructed (see figure 1 for a schematic representation of the tomosynthesis system). DBT images are the grayscale

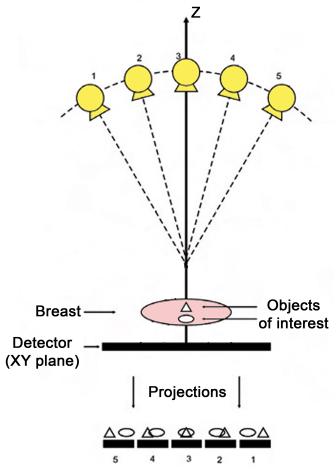


Figure 1: Tomosynthesis system in yz plane.

representation of the attenuation coefficients of each voxel of the breast. If we suppose a monochromatic X-ray source, the continuous mathematical model of the image formation process is described by the Beer's law that relates the measured values $\bar{g}_i^{(\theta)}$ at each pixel i of the detector, for a fixed angle θ, with the attenuation coefficient μ for each position $\mathbf{w}$ of the object:

$$\bar{g}_i^{(\theta)} = \mathtt{exp}\left(-\int_{L_\theta} \mu(\mathbf{w})dl\right) + \bar{\eta}_i^{(\theta)}, \quad i = 1\dots N_p, \theta = 1,\dots N_\theta, \tag{1}$$

where:

- N_p is the number of pixels in the detector (N_p is of the order of millions in the real systems);

- N_θ is the number of angles (common values are $10 \leq N_\theta \leq 25$ in the real systems);
- L_θ is the line followed by the X-ray beam through the object;
- $\mu(\mathbf{w})$ is the linear attenuation coefficient, at the position $\mathbf{w} = (x, y, z)$, depending on the material in the object and characterizing the structures inside the object. We remind that denser materials, such as calcifications, have a greater attenuation coefficient;
- $\bar{\eta}_i^{(\theta)}$ is the noise measured at the detector (pixel i, angle θ) and it includes scattering and electronic noise.

The discretization of equation (1) is:

$$\bar{g}_i^{(\theta)} = \mathtt{exp}\left(-\sum_{l=1}^{N_v} m_{il}^{(\theta)} \mu_l\right) + \bar{\eta}_i^{(\theta)} \tag{2}$$

where:

- N_v is the number of voxels (few billions in the real systems) in the discretized 3D object;
- $m_{il}^{(\theta)}$ is the element of a matrix $M^{(\theta)}$ obtained with the ray-tracing technique proposed by Siddon.

If we take the negative logarithm of (2) and we reorder all the resulting projections and noise elements in vectors g and η of length $N_p \cdot N_\theta$, we obtain the matrix equation:

$$g = Mf + \eta \tag{3}$$

where the matrix $M = m_{il}^{(\theta)}$ is sparse with size $(N_p \cdot N_\theta) \cdot N_v$ (in our case $N_p \cdot N_\theta < N_v$), and f is the vector with elements $\mu_l, l = 1, \ldots N_v$. Iterative statistical reconstruction algorithms, that maximize the similarity between the computed and measured projections at each iteration and enables the introduction of priors have some advantages over the traditional Filtered Back-Projection (FBP) method in the noise reduction and in the identification of the object borders. Investigation of iterative algorithms derived from complete data tomography and applied to DBT, such as Maximum Likelihood (ML) or Algebraic Iterative Algorithms (ART), can be found in [1].
Tomosynthesis reconstruction is an ill-posed problem both for the ill posedness of the continuous projection operator and for the data incompleteness, that causes infinite solutions to the underdetermined linear system (3). For this reason, the idea of using a regularization operator has been introduced in [3], with the double purpose of loosening up the consistency with the data and of selecting an image with the prescribed regularity. The regularization function makes assumption on the reconstructed image and forces the choices of one of the infinite possible solutions.
Recently, the compressed sensing theory [4] has been used in Computed Tomography (CT). If the image is supposed sparse in some domain, the minimization of the 1-norm in that domain guarantees the sparsity of the solution. For breast images, where the interest is to identify microcalcifications and/or masses, the image gradient is supposed to be sparse and the Total Variation (TV) regularization function has been succesfully employed [3]. In this case, the minimization problem can have a constrained formulation:

$$\min_f TV(f) \quad s.t. \quad \|Mf - g\|_2^2 \leq \sigma \tag{4}$$

or an equivalent uncostrained formulation:

$$\min_f \|Mf - g\|_2^2 + \lambda TV(f). \tag{5}$$

where the TV function is defined as [2, 6]:

$$TV(x) = \int_\Omega |\nabla x| dx \tag{6}$$

where Ω is the image domain and $|\cdot|$ is the $L2$ norm. Since the TV is not differentiable, usually it is substituted by a smooth differentiable function. In deblurring and/or denoising applications a small parameter β is often added and a smoothed version of the TV function is obtained as:

$$TV_\beta(f) = \int_\Omega |\nabla f + \beta| df \tag{7}$$

with β a small positive value. In this paper we use this last strategy and $TV_\beta(f)$ is considered in place of $TV(f)$ in the following.
Some iterative algorithms for the solution of problem (4) or (5) applied to the reconstruction of 3D tomographic images have been investigated in literature. All the cited algorithms are first order algorithms, since they use only the gradient information of the objective function. We consider two iterative algorithms for the solution of (5): the Scaled Gradient projection (SGP) method [5] and the Fixed Point (FP) [6] method. The SGP method finds a nonnegative solution of the minimization problem (5). It is a gradient-like method accelerated by using a scaling matrix and the Barzilai-Borwein rules for the choice of the steplength. This algorithm has been recently proposed in imaging applications with very good results in terms of efficiency and precision . The FP method is a Newton-like method for the solution of the minimization problem (5), whose descent step is computed by solving a linear system. The coefficient matrix is an approximation of the Hessian of the objective function $\mathcal{J}(f)$. The FP algorithm has been proposed for the solution of image denoising and image deblurring TV regularized problems due to its fast convergence.
Some numerical results on a digital phantom used in DBT simulations showed that both methods give very good reconstructions in few iterations.

References

[1] T. Wu, R. H. Moore, and al. A comparison of reconstruction algorithms for breast tomosyntesis. *Medical Physics*, 31(9):2636–2647, 2004.

[2] L. Rudin and S. Osher and E. FatemiNonlinear total variation based noise removal algorithms. *Phys. D*, 60:259-268, 1992.

[3] E. Y. Sidky, X. Pan, I. S. Reiser, and R. M. Nishikawa. Enhanced imaging of microcalcifications in digital breast tomosynthesis through improved image-reconstruction algorithms. *Medical Physics*, 36(11):4920–4932, 2009.

[4] D. L. Donoho. Compressed sensing. *IEEE Trans. Inf. Theory*, 52:289–306, 2006.

[5] J. Nocedal and S. J. Wright. *Numerical optimization*. Springer-Verlag New York, Inc., 1999.

[6] C. R. Vogel. *Computational Methods for Inverse Problems*. SIAM, Philadelphia, PA, USA, 2002.

A modified Nyström method for a BIE related to the exterior Neumann problem on domains with corners

Concetta Laurita
Università degli Studi della Basilicata
via dell'Ateneo Lucano, 10 85100 - Potenza Italy
concetta.laurita@unibas.it

We are concerned with the numerical solution of the exterior Neumman problem for the Laplace equation in two-dimensional domains with piecewise smooth boundaries. Let $\Omega \subset \mathbb{R}^2$ be an open, bounded simply connected domain, with a piecewise smooth Lipschitz boundary Γ. We shall assume that the boundary curve Γ contains r corner points $P_1, \ldots, P_r$ and is otherwise smooth. We consider the problem

$$\begin{array}{ll} \Delta u = 0, & \text{in } \mathbb{R}^2 \setminus \bar{\Omega}, \\ \dfrac{\partial u}{\partial n} = f, & \text{on } \Gamma, \\ |u(x)| = o(1), & \text{as } |x| \to \infty, \end{array} \quad , \tag{1}$$

where n denotes the unit normal to the boundary Γ, directed into the exterior $\mathbb{R}^2 \setminus \bar{\Omega}$, and f is a sufficiently smooth function satisfying

$$\int_\Gamma f ds = 0.$$

A boundary integral equation (BIE) formulation of the exterior Neumann problem (1) is obtained by using the single layer representation of the potential u, i.e.

$$u(x) = -\int_\Gamma \phi(y) \log|x-y| dS(y), \quad x \in \mathbb{R}^2 \setminus \bar{\Omega}, \tag{2}$$

where $|x-y|$ is the Euclidean distance between x and y, $dS(y)$ is the element of arc length and ϕ is the so called single-layer density function. The single layer potential (2) is a solution of (1) provided that the density ϕ is a solution of the integral equation

$$-\pi\phi(x) - \int_\Gamma \frac{\partial}{\partial n(x)} \log|x-y| \phi(y) dS(y) = f(x), \quad x \in \Gamma, \tag{3}$$

and in addition satisfies

$$\int_\Gamma \phi(y) dS(y) = 0.$$

By applying a suitable decomposition of the boundary Γ, the BIE (3) can be converted into a system of r integral equations of the second kind with fixed singularities of Mellin type. Smoothing strategies are used for dealing with the singularities as well as a suitable "modified" Nyström type method, recently proposed in [1], is applied in order to approximate the solution of this system. The stability and the convergence of the numerical procedure are proved in L^2 spaces and error estimates are also given. Moreover, some numerical results show the effectiveness of the method.

References

[1] De Bonis, M. C. and Laurita, C. 2016 *A modified Nyström method for integral equations with Mellin type kernels*. J. Comp. Appl. Math. 296, 512–527.

A Nyström method for Fredholm integral equations on the real semiaxis with nonstandard weights

Incoronata Notarangelo
Università degli Studi della Basilicata
viale dell'Ateneo Lucano 10, 85100 - Potenza Italy
incoronata.notarangelo@unibas.it

Giuseppe Mastroianni
Università degli Studi della Basilicata
viale dell'Ateneo Lucano 10, 85100 - Potenza Italy
giuseppe.mastroianni@unibas.it

Gradimir V. Milovanović
Mathematical Institute of the Serbian Academy of Sciences and Arts
Kneza Mihaila 36, 11000 - Beograd Serbia
gvm@mi.sanu.ac.rs

We propose a Nyström-type method to approximate the solution of integral equations of the form

$$f(x) - \mu \int_0^{+\infty} k(x,y) f(y) w(y)\, \mathrm{d}y = g(x)\,, \quad x \in (0, +\infty),$$

where $\mu \in \mathbb{R}$,

$$w(y) = \mathrm{e}^{-y^{-\alpha} - y^{\beta}}\,, \quad \alpha > 0\,,\ \beta > 1\,,$$

the given functions k and g can grow exponentially with respect to their arguments, when they approach to 0^+ and/or $+\infty$ [6]. This method is based on a "truncated" Gaussian rule w.r.t. the nonstandard weight w.
Since the solution of this kind of equations can increase exponentially for $x \to 0^+$, the methods based on the weighted polynomial approximation with Laguerre-type weights are not suitable in this case. So, a first difficulty is to choose proper function spaces where these equations can be studied. To this aim, we introduce another exponential weight u and new function spaces C_u with weighted uniform metric. We prove that the proposed method is stable and convergent in this metric, using our recent results on polynomial approximation with the weight u [2, 3, 4] and related Gaussian rules [5].
Moreover, the weight w is nonclassical and the coefficients of the three terms recurrence relation for the related orthogonal polynomials are not explicitly known. Therefore, another main difficulty is to construct the coefficients of the Gaussian rule related to the weight w. For the computation of the zeros and the Christoffel number we use a procedure given in [5] and the Mathematica package `OrthogonalPolynomials` [1].
Finally, we give a priori error estimates and show some numerical examples, including a comparison with other Nyström methods.

References

[1] Cvetković, A.S. and Milovanović, G.V. 2004 *The Mathematica Package "OrthogonalPolynomials"*, Facta Univ. Ser. Math. Inform. 9, 17–36.

[2] Mastroianni, G. and Notarangelo, I. 2013 *Embedding theorems with an exponential weight on the real semiaxis*, Electronic Notes in Discrete Mathematics 43, 155–160.

[3] Mastroianni, G., Notarangelo, I. and Szabados, J. 2013 *Polynomial inequalities with an exponential weight on* $(0, +\infty)$, Mediterranean Journal of Mathematics 10, no. 2, 807–821.

[4] Mastroianni, G. and Notarangelo, I. 2014 *Polynomial approximation with an exponential weight on the real semiaxis*, Acta Mathematica Hungarica 142, 167–198.

[5] Mastroianni, G., Milovanović, G.V. and Notarangelo, I. 2014 *Gaussian quadrature rules with an exponential weight on the real semiaxis*, IMA Journal of Numerical Analysis 34, 1654–1685.

[6] Mastroianni, G., Milovanović, G.V. and Notarangelo, I. *A Nyström method for a class of Fredholm integral equations on the real semiaxis*, submitted.

A new numerical method for mixed boundary value problems on domains with corners

Luisa Fermo
Università degli Studi di Cagliari
viale Merello, 92 09123 - Cagliari Italy
fermo@unica.it

Concetta Laurita
Università degli Studi della Basilicata
via dell'Ateneo Lucano, 10 85100 - Potenza Italy
concetta.laurita@unibas.it

This talk deals with the numerical solution of mixed Dirichlet-Neumann boundary value problems for the Laplace equation

$$\begin{cases} \Delta u(P) = 0, & P \in D \\ u(P) = f_D(P), & P \in \Sigma_D \\ \dfrac{\partial u(P)}{\partial n_P} = f_N(P), & P \in \Sigma_N \end{cases}$$

where D is a simply connected bounded region in the plane with a piecewise smooth-boundary $\Sigma = \bar{\Sigma}_D \cup \bar{\Sigma}_N$, f_D and f_N are given functions on Σ_D and Σ_N, respectively and n_P is the inner normal vector to Σ_N at P. Following a well-known theory, we represent the solution u as the single layer potential

$$u(A) = \int_\Sigma \Psi(Q) \log|A - Q| \, d\Sigma_Q, \quad A \in D$$

where Ψ denotes the unknown single layer density function satisfying the following system

$$\begin{cases} \displaystyle\int_\Sigma \Psi(Q) \log|P - Q| \, d\Sigma_Q = f_D(P), & P \in \Sigma_D \\ \pi\Psi(P) + \displaystyle\int_\Sigma \Psi(Q) \frac{\partial}{\partial n_P} \log|P - Q| \, d\Sigma_Q = f_N(P), & P \in \Sigma_N. \end{cases}$$

The latter is characterized by a boundary integral equation of the second kind having Mellin-type integral operators. Hence, for its numerical solution, we propose a method of Nyström type based on Legendre quadrature formulas which are "modified" around the corners. We examine the stability of the proposed method and discuss the convergence, which is accelerate by using regularized technique. Moreover, we illustrate numerical tests showing the efficiency of the new approach.

Recent kinetic models and their hydrodynamic limits - Part I

PROPOSERS

Marzia Bisi
Università degli Studi di Parma
Parco Area delle Scienze 53/A, 43124 - Parma Italy
marzia.bisi@unipr.it

Silvia Lorenzani
Politecnico di Milano
Via E. Bonardi 9, 20133 - Milano Italy
silvia.lorenzani@polimi.it

SPEAKERS

Laurent Desvillettes (keynote)
Université Paris Diderot
desvillettes@math.univ-paris-diderot.fr

Luigi Barletti
Università di Firenze
luigi.barletti@unifi.it

Marzia Bisi
Università degli Studi di Parma
marzia.bisi@unipr.it

Orazio Muscato
Università di Catania
muscato@dmi.unict.it

Valeria Ricci
Università di Palermo
valeria.ricci@unipa.it

In recent years, the kinetic approach is playing an important role not only in the description of dynamics of rarefied gases, following the classical Boltzmann lines, but also in modelling systems composed by many elementary entities, which exchange between themselves and/or with a host medium some quantities carried by them. Some of these new applications of kinetic theory concern reactive mixtures of polyatomic gases or plasmas, granular materials, wealth distribution in a simple market economy, opinion formation, biological propagation phenomena, vehicular traffic, crowd dynamics. In all of these generalizations of Boltzmann equations, the crucial point is the construction of proper "collision" rules, since interactions are usually not conservative as in the classical elastic case, and may also be influenced by external effects. Indeed, there are substantial differences between the collision mechanism of particles and human interactions: in social sciences usual mechanical conservations are lacking, and random (unpredictable) effects

might play a crucial role; moreover, in classical Boltzmann theory the velocity variable ranges over the whole space, while in socio–economic problems the kinetic variable must fulfill some proper bounds (for instance, in a market economy the amount of wealth has to be non–negative, if debts are not allowed). However, kinetic approach seems to be very promising, since it is able to identify some universal behaviors and asymptotic profiles, which turn out to depend only on some basic features of the interaction rules, neglecting all other details. The main goal of this minisymposium is to spread recent (analytical and numerical) advances on kinetic models for systems with non–conservative interactions, and also on the asymptotic procedure leading from the kinetic level to suitable hydrodynamic equations for the major macroscopic fields. In Part I we focus the attention mainly on kinetic and macroscopic equations for reacting gas mixtures, and on their possible applications to physical problems as diffusion of sprays, electron transport in graphene or in silicon carbide semiconductors. Then, Part II is devoted to models for biological or social sciences, as kinetic cellular models for tumor–immune system interactions, modelling and simulation of social crowd dynamics, kinetic description of vehicular traffic.

Some remarks on Boltzmann's H-theorem

Laurent Desvillettes
Université Paris-Diderot
IMJ-PRG, Batîment Sophie Germain, 11, Rue de Saint-Denis, 45650 - Saint-Jean le Blanc
France
desvillettes@math.univ-paris-diderot.fr

We consider in this talk collision kernels $Q := Q(f)$ arising in the kinetic theory of gases and plasmas, such as the Boltzmann operator for monoatomic or polyatomic rarefied gases, the Landau operator for plasmas, and extensions of those operators appearing in a relativistic context, or in the theory of semiconductors.

All these operators have in common an entropy structure, that is $D(f) := \int Q(f) \ln f \leq 0$ (some variant of this inequality can hold, for example in cases in which the Pauli exclusion principle has to be taken into account). This is sometimes called the first part of Boltzmann's H-theorem.

The second part of Boltzmann's H-theorem is concerned with the case of equality in the inequality $D(f) \leq 0$. It states that $D(f) = 0$ if and only if f belongs to a specific set of functions. In the case of the usual Boltzmann kernel, those functions are the Maxwellians, that is, $\ln f = a + b \cdot v + c|v|^2$.

We revisit the proof of this statement and provide extensions in cases when Q is not conserving the classical kinetic energy $|v|^2/2$ but some more complicated quantity. We also explain in which sense this statement is robust, using recent results on the Landau equation with Coulomb interaction.

A Hybrid Classical-Quantum Diffusive Model for Charge Transport in Graphene

Luigi Barletti
DIMAI - Università degli Studi di Firenze
viale Morgagni, 67/A 50134 - Firenze Italy
luigi.barletti@unifi.it

Claudia Negulescu
IMT - Université Paul Sabatier
18, Route de Narbonne, 31062 - Toulouse France
claudia.negulescu@math.univ-toulouse.fr

Electrons on a graphene sheet, in presence of sharp potential steps or barriers, undergo remarkable phenomena, such as highly-selective angle-dependent transmission coefficient [6] and negative electronic refraction index [4]. These phenomena are intimately related to the chiral nature of electronic tunneling in graphene and to the Dirac-like conical dispersion relation [3]. However, a fully-quantum description of the electron dynamics is only important in a small region around the steep potential while, elsewhere, the semiclassical equations of motion provide an excellent approximation.
In this contribution we derive a quantum-diffusive models of stationary electron transport in graphene, where a quantum region (an asymptotically thin strip around the potential step) is coupled through the quantum scattering data to a classical region, described in terms of semiclassical diffusive equations [1].
Our approach is based on a seminal paper by N. Ben Abdallah [2], concerning the quantum-kinetic coupling, successively extended by P. Degond and A. El Ayyad [5] to the quantum-diffusive coupling. The original approach was developed for scalar particles with standard (i.e. parabolic) dispersion relation.
However, the application of the theory to electrons in graphene is far from being trivial because of the possible exchanges between upper-cone and lower-cone electron states and (as soon as statistical considerations come into play) because of unbounded negative energies, requiring the use of Fermi-Dirac statistics and the description of lower-cone electrons in terms of holes.
Assuming the steep potential variations to be along a single direction, we first extend the construction of Ref. [2] to the case of electrons in graphene, obtaining a stationary, hybrid kinetic-quantum model, represented by two semiclassical transport equations coupled by quantum transmission conditions through a one-dimensional interface. Then, following Ref. [5], we take the diffusive limit of such quantum-kinetic model, by introducing a suitable boundary layer corrector and applying the Chapman-Enskog procedure. A key step in the derivation of the diffusive limit is the introduction of a boundary layer corrector defined in terms of the solutions of a two-sided vector Milne problem. Here, however, because of the chirality degree of freedom, the construction of the boundary corrector leads to the discussion of a system of four (instead of one) half-space, half-range Milne problems.
In this way, a stationary, hybrid diffusive-quantum model is obtained which is constituted

by two semiclassical drift-diffusion equations coupled by diffusive transmission conditions, expressed as a system of constraints relating the upper/lower-left/right chemical potentials across the quantum interface. Finally, by means of a Maxwell-Boltzmann approximation of the Fermi-Dirac distribution, such constraints are translated into a more explicit constraints on densities. In this way, the quantum information is concentrated into four constants appearing in the diffusive transmission conditions, namely, the asymptotic densities far from the interface, that are obtained from the Milne system.

References

[1] Barletti, L. 2014 *Hydrodynamic equations for electrons in graphene obtained from the maximum entropy principle*. J. Math. Phys. 55, 083303.

[2] Ben Abdallah, N. 1998 *A hybrid kinetic-quantum model for stationary electron transport in a resonant tunneling diode*. J. Stat. Phys. 90, 627–662.

[3] Castro Neto, A. H., Guinea, F., Peres, N. M. R., Novoselov, K. S. and Geim, A. K. 2009 *The electronic properties of graphene*. Rev. Mod. Phys. 81, 109–162.

[4] Cheianov, V.V., Fal'ko, V. and Altshuler, B.L. 2007 *The focusing of electron flow and a Veselago lens in graphene*. Science 315, 252–1255.

[5] P. Degond, P. and El Ayyad, A. 2002 *A coupled Schrödinger Drift-Diffusion model for quantum semiconductor device simulations*. J. Comput. Phys. 181, 222–259.

[6] Katsnelson, M. I., Novoselov, K. S. and Geim, A.K. 2006 *Chiral tunnelling and the klein paradox in graphene*. Nature Physics 2, 620–625.

Hydrodynamic limits of kinetic equations for polyatomic gases

Marzia Bisi
Università degli Studi di Parma
Parco Area delle Scienze, 53/A 43124 - Parma, Italy
marzia.bisi@unipr.it

Giampiero Spiga
Università degli Studi di Parma
Parco Area delle Scienze, 53/A 43124 - Parma, Italy
giampiero.spiga@unipr.it

Tommaso Ruggeri
Università degli Studi di Bologna
Via Saragozza, 8 40123 - Bologna, Italy
tommaso.ruggeri@unibo.it

It is well known that gases involved in physical applications, for instance in simple dissociation and recombination problems or in the evolution of dust in the atmosphere, are usually composed of polyatomic particles. In kinetic theory, non–translational degrees of freedom of polyatomic gases are taken into account through a suitable internal energy variable. Specifically, two different Boltzmann–type approaches have been proposed in the literature: the one developed in [4], in which the gas is endowed with a set of discrete energy levels, and the one presented in [3], in which the internal energy is assumed to be a continuous function. In both cases equilibrium distributions are of Maxwellian type, affected by internal energies through suitable "partition functions", and the capability of these models of reproducing some basic features of polytropic or non–polytropic gases will be commented on.
A consistent BGK model that reproduces correct equilibria, collision invariants, and H-theorem of the original Boltzmann equations with discrete energy has been recently proposed [1]. We will present an asymptotic Chapman–Enskog analysis of such a relaxation model in order to achieve consistent fluid–dynamic Navier–Stokes equations for the macroscopic fields. Among the various transport coefficients, emphasis will be given to the "dynamical pressure" [2], which characterizes molecules with non–translational degrees of freedom, and the comparison with analogous hydrodynamic results recently derived [5] for the model with continuous internal energy will be discussed.

References

[1] Bisi, M. and Càceres, M.J. 2016 *A BGK relaxation model for polyatomic gas mixtures* Commun. Math. Sci. 14, 297–325.

[2] Bisi, M. and Spiga, G. *On kinetic models for polyatomic gases and their hydrodynamic limits*. Ricerche di Matematica (in press).

[3] Desvillettes, L., Monaco, R. and Salvarani, F. 2005 *A kinetic model allowing to obtain the energy law of polytropic gases in the presence of chemical reactions*. Europ. J. Mech. B/ Fluids 24, 219–236.

[4] Groppi, M. and Spiga, G. 1999 *Kinetic approach to chemical reactions and inelastic transitions in a rarefied gas*. J. Math. Chem. 26, 197–219.

[5] Pavic, M., Ruggeri, T. and Simic, S. 2013 *Maximum entropy principle for rarefied polyatomic gases*. Phys. A 392, 1302–1317.

A hierarchy of hydrodynamic models for silicon carbide semiconductors

Orazio Muscato
Dipartimento di Matematica e Informatica, Università degli Studi di Catania
viale A. Doria, 6 95125 - Catania Italy
muscato@dmi.unict.it

Vincenza Di Stefano
Dipartimento di Matematica e Informatica, Università degli Studi di Catania
viale A. Doria, 6 95125 - Catania Italy
vdistefano@dmi.unict.it

Silicon Carbide (SiC) is a potential leader in high-power and high temperature electronics due to the favorable combination of several material properties such as the wide bandgap, the high thermal conductivity, the high breakdown field. Although the performances of SiC are very promising, SiC devices may suffer from severe self-heating effects which impose a limitation on both the output power and the power density of the devices. Self heating results in a higher lattice temperature in the transistor channel which can significantly deteriorate the current-voltage characteristics because of the reduction in the device parameters such as mobility and electron saturation velocity. For these reasons, electro-thermal simulations are necessary in order to predict the behaviour of such devices. The natural framework for describing electro-thermal transport phenomena is based on the Bloch-Boltzmann-Peierls kinetic equations (BBP) for the coupled system formed by the electrons and the phonons, together with the Poisson equation. The fundamental approach is to solve the BBP equations, but this is not an easy task also from the numerical point of view, because they form a set of partial integro-differential equations. In order to study the electro-thermal transport, a good engineering-oriented approach is to introduce hydrodynamic models, which are obtained by taking the moments of the BBP equations and by using a suitable truncation procedure.
Closure relations for the higher order moments and production terms involving the electron-phonon scattering have been obtained by means of the Maximum Entropy Principle [1]. By introducing a diffusive scaling, an Energy Transport model (ETM) has been derived, where the transport coefficients do not contain any fitting parameters, but only the physical constants as the coupling ones and the phonon energies that are present in the transition rate probabilities of the scatterings between the electrons and phonons. In the limit case when the electrons and phonons have the same temperature, the ETM reduces to the standard non-isothermal Drift Diffusion model. The low-field mobility we have obtained in this case, shows a good agreement with the experimental data.

References

[1] O. Muscato and V. Di Stefano, *Electrothermal transport in silicon carbide semiconductors via a hydrodynamic model*, SIAM J. APPL. MATH., 75(4), 1941–1964, (2015)

Validation of models for sprays

Valeria Ricci
Università degli Studi di Palermo, Dipartimento di Matematica e Informatica
via Archirafi, 34 90123 - Palermo Italy
valeria.ricci@unipa.it

We consider complex fluids consisting of a dispersed phase (solid particles or liquid droplets) immersed in a gas.
A class of models describing the dynamics of such a kind of systems is given by a system of partial differential equations where a kinetic equation, describing the dispersed phase, is coupled to a fluid equation for the background gas. The coupling is given by the drag force exerted by the gas on the dispersed phase.
Within this class, we shall analyse the case where the kinetic equation is a Vlasov-type equation and the fluid equation are of Stokes or Navier-Stokes type.
We shall discuss the validation problem for this class of models, i.e. the derivation of the equations of the model from evolution equations given on a scale which can be considered "microscopic" with respect to the final one; in particular we shall analyse the difficulty of dealing with a particle model for the system ([1, 2]), and the (formal) derivation of the Vlasov-(Navier-)Stokes model from a multiphase Boltzmann model in suitables asymptotics ([3]).
The results have been obtained in collaboration with E.Bernard, L.Desvillettes, F.Golse.

References

[1] Desvillettes, L. and Golse, F. and Ricci, V. 2008 *The mean-field limit for solid particles in a Navier-Stokes flow* . J. Stat. Phys., 131, 941–967

[2] Ricci, V. 2015 *Modelling of systems with a dispersed phase: "measuring" small sets in the presence of elliptic operators*, to appear in From Particle Systems to Partial Differential Equations III, Springer Proceedings in Mathematics & Statistics, in press.

[3] Bernard, E. and Desvillettes, L. and Golse, F. and Ricci, *A derivation of the Vlasov-Navier-Stokes model for aerosol flows from kinetic theory*, preprint.

Recent kinetic models and their hydrodynamic limits - Part II

PROPOSERS

Marzia Bisi
Università degli Studi di Parma
Parco Area delle Scienze 53/A, 43124 - Parma Italy
marzia.bisi@unipr.it

Silvia Lorenzani
Politecnico di Milano
Via E. Bonardi 9, 20133 - Milano Italy
silvia.lorenzani@polimi.it

SPEAKERS

Giacomo Dimarco
Università di Ferrara
giacomo.dimarco@unife.it

Livio Gibelli
Politecnico di Torino
livio.gibelli@polito.it

Maria Groppi
Università di Parma
maria.groppi@unipr.it

Andrea Tosin
Politecnico di Torino
andrea.tosin@polito.it

Fiammetta Conforto
Università di Messina
fiammetta.conforto@unime.it

Silvia Lorenzani
Politecnico di Milano
silvia.lorenzani@polimi.it

In recent years, the kinetic approach is playing an important role not only in the description of dynamics of rarefied gases, following the classical Boltzmann lines, but also in modelling systems composed by many elementary entities, which exchange between themselves and/or with a host medium some quantities carried by them. Some of these new applications of kinetic theory concern reactive mixtures of polyatomic gases or plasmas, granular materials, wealth distribution in a simple market economy, opinion formation, biological propagation phenomena, vehicular traffic, crowd dynamics. In all of these generalizations of Boltzmann equations, the crucial point is the construction of

proper "collision" rules, since interactions are usually not conservative as in the classical elastic case, and may also be influenced by external effects. Indeed, there are substantial differences between the collision mechanism of particles and human interactions: in social sciences usual mechanical conservations are lacking, and random (unpredictable) effects might play a crucial role; moreover, in classical Boltzmann theory the velocity variable ranges over the whole space, while in socio–economic problems the kinetic variable must fulfill some proper bounds (for instance, in a market economy the amount of wealth has to be non–negative, if debts are not allowed). However, kinetic approach seems to be very promising, since it is able to identify some universal behaviors and asymptotic profiles, which turn out to depend only on some basic features of the interaction rules, neglecting all other details. The main goal of this minisymposium is to spread recent (analytical and numerical) advances on kinetic models for systems with non–conservative interactions, and also on the asymptotic procedure leading from the kinetic level to suitable hydrodynamic equations for the major macroscopic fields. In Part I we focus the attention mainly on kinetic and macroscopic equations for reacting gas mixtures, and on their possible applications to physical problems as diffusion of sprays, electron transport in graphene or in silicon carbide semiconductors. Then, Part II is devoted to models for biological or social sciences, as kinetic cellular models for tumor–immune system interactions, modelling and simulation of social crowd dynamics, kinetic description of vehicular traffic.

Macroscopic models of collective motion with repulsion

Giacomo Dimarco
Università degli Studi di Ferrara
Via Machiavelli, 30 44121 - Ferrara Italy
giacomo.dimarco@unife.it

Pierre Degond
Imperial College, London
London SW7 2AZ, United Kingdom
p.degond@imperial.ac.uk

We study a system of self-propelled particles which interact with their neighbors via alignment and repulsion. The particle velocities result from self-propulsion and repulsion by close neighbors. The direction of self-propulsion is continuously aligned to that of the neighbors, up to some noise. A continuum model is derived starting from a mean-field kinetic description of the particle system. It leads to a set of non conservative hydrodynamic equations. We provide a numerical validation of the continuum model by comparison with the particle model. We also provide comparisons with other self-propelled particle models with alignment and repulsion.

A Kinetic Theory approach to behavioral social crowds

Livio Gibelli
Politecnico di Torino
Corso Duca degli Abruzzi, 24 10129 - Torino Italy
livio.gibelli@polito.it

The study of human crowds is a challenging interdisciplinary research field which is motivated not only by its theoretical interest but also by the potential societal benefits [4]. Indeed the realistic modelling and simulation of the pedestrian behavior can be used to gain insights into possible problems regarding the evacuation of public buildings, aircrafts and ships early in their planning and/or understanding of how to guide crowd in different situations.
Most of the existing crowd models are developed at the microscopic [5] and macroscopic [6] scales. Microscopic models assume that the dynamics of the crowd emerges from the movement of individuals. Accordingly, its state is predicted by specifying the microscopic state of pedestrians, namely positions and velocities, and defining their interactions rules. Mathematical models are thus stated in terms of systems of ordinary differential equations. In contrast, macroscopic models focus on the crowd as a whole and are in the form of balance equations for aggregate observables, such as mass and/or momentum, closed by phenomenological assumptions. Mesoscopic models are situated at an intermediate level. The crowd is described by means of a probability distribution function over the microscopic state of individuals. Interactions are modeled at the micro-scale, while mean quantities are obtained by weighted moments of the aforesaid probability distribution. The space and time evolution of the latter is usually given by integro-differential equations. Microscopic models may provide realistic results but keeping track of the individual state of each walker leads to numerical simulations which are computationally demanding. Moreover, the results obtained from such approach may be difficult to interpret in the absence of a higher level model, that is, it may be difficult or nearly impossible to use data from microscopic observations to predict what happens in a similar but different situation. On the other hand, the heterogeneous behavior of walkers gets lost in the averaging process needed to derive macroscopic models which, therefore, totally disregard this important feature. Although more work is certainly needed, the mesoscopic modelling of human crowds is promising in that it permits to capture both the behavioral and social features of the pedestrians behavior while keeping the computing effort at a reasonable level.
The talk presents a crowd mesoscopic model based on the kinetic theory of active particles. Such a theory has been specifically developed to model the dynamics of systems composed of many living interacting entities and combines methods of classical kinetic theory with theoretical tools of game theory. The model has been initially proposed in [1] for describing a crowd in unbounded domains, and further developed in [2] to account for interactions with walls and in [3] to improve its capability to reproduce the empirical evidence.
In homogeneous steady conditions, the model provides a reasonable fundamental density-velocity diagram, namely the predictions of the mean speed of walkers as a function of the

density are consistent with empirically data. In non-homogeneous conditions, it depicts well known collective emerging behaviors, such as lane formation in pedestrian counter flow and the increasing of the evacuation time under stressful conditions. Furthermore, the model can account for the onset and propagation of social behaviors. This capability is particularly important in the evacuation dynamics, where panic conditions, originated in a restricted area, can rapidly be transferred to the whole crowd and may generate highly dangerous situations.

References

[1] Bellomo N, Bellouquid A, Knopoff D. From the micro-scale to collective crowd dynamics. Multiscale Modelling Simulations 2013; 11: 943-963.

[2] Bellomo N, Gibelli L. Toward a behavioral-social dynamics of pedestrian crowds. Math. Models Methods Appl. Sci. 2015; 25: 2417-2437.

[3] Bellomo N, Gibelli L. Behavioral crowds: Modeling and Monte Carlo simulations toward validation. Comp. & Fluids, 2016; in press.

[4] Cristiani E, Piccoli B, Tosin A. Multiscale Modeling of Pedestrian Dynamics. Springer; 2014.

[5] Helbing D. Traffic and related self-driven many-particle systems. Rev. Modern Phys. 2001; 73: 1067-1141.

[6] Hughes RL. The flow of human crowds. Annu. Rev. Fluid Mech. 2003; 35: 169-182.

Dynamics of tumor–immune system interaction: a kinetic approach

Maria Groppi
Università degli Studi di Parma
Parco Area delle Scienze, 53/A 43124 - Parma Italy
maria.groppi@unipr.it

Martina Conte
Università degli Studi di Parma
Parco Area delle Scienze, 53/A 43124 - Parma Italy
martina.conte1@studenti.unipr.it

Giampiero Spiga
Università degli Studi di Parma
Parco Area delle Scienze, 53/A 43124 - Parma Italy
giampiero.spiga@unipr.it

A kinetic model describing the competition between tumor cells and immune system is investigated. The starting point is represented by the kinetic equations for the evolution of dominance in populations of interacting organisms, taking nonconservative effects of proliferation and destruction into account [2]. Four interacting populations are considered, representing, respectively, tumors cells, cells of the host environment, cells of the immune system, and interleukines, which are capable to modify the tumor-immune system interaction, and to contribute to destroy tumor cells. The internal state variable (activity) measures the capability of a cell of prevailing in a binary interaction.
A closed set of autonomous ODEs is then derived by a moment procedure, representing a sort of macroscopic continuity equations in the sense of kinetic theory. Under very reasonable assumptions on the microscopic interaction parameters, two three-dimensional reduced systems of ODEs are obtained in a partial quasi-steady state approximation. In the first approximation the host environment plays the role of background; in the second one this role is assumed by the interleukines. The qualitative analysis of these evolution problems is then performed in the framework of the theory of dynamical systems. Essential steps are determination of fixed points, as stationary living conditions of the considered organism, and of their stability, as well as possible occurrence of bifurcations for varying parameters. The analysis shows that the reduced system describing interactions between tumor, immune system and interleukines can be investigated in the framework of the theory of the asymptotically autonomous differential systems [3], and then its asymptotic behaviours can be deduced from an easier two dimensional limit system. An important feature of the second reduced system for the interactions between tumor, immune system and host environment is the presence, also in this context, of a backward bifurcation, which is usually related to epidemic models [1].

References

[1] Hadeler K.P., Castillo-Chavez C. 1995 *A core group model for disease transmission.* Math. Biosci. 128, 41–55.

[2] Iori M., Nespi G., Spiga G. 1999 *Analysis of a kinetic cellular model for tumor–immune system interaction.* Math. Comput. Modelling 29, 117–129.

[3] Thieme H.R. 1993 *Asymptotically autonomous differential equations in the plane.* Rocky Mt. J. Math. 24, 351–380.

A Boltzmann-type kinetic approach to the study of vehicular traffic

Andrea Tosin
Politecnico di Torino
Corso Duca degli Abruzzi, 24 10129 - Torino Italy
andrea.tosin@polito.it

In this talk I will present a kinetic approach to the modelling of vehicular traffic. Sticking to the idea that the macroscopic characteristics of the flow of vehicles are ultimately due to microscopic interactions among cars, the approach consists in implementing a probabilistic description of speed changes in a Boltzmann-type collisional operator.
In particular, I will discuss how this approach allows one to study the fundamental diagrams of traffic, possibly also considering a heterogeneous composition of the flow of vehicles, up to some hydrodynamic/Fokker-Planck limits.

This is a joint work with: L. Fermo (University of Cagliari), P. Freguglia (University of L'Aquila), M. Herty (RWTH Aachen University), G. Puppo (University of Insubria), M. Semplice (University of Turin), G. Visconti (University of Insubria).

References

[1] Fermo, L. and Tosin, A. 2014 *Fundamental diagrams for kinetic equations of traffic flow*. Discrete Contin. Dyn. Syst. Ser. S, 7(3), 449–462.

[2] Freguglia, P. and Tosin, A. 2016 *Proposal of a risk model for vehicular traffic: A Boltzmann-type kinetic approach*. Commun. Math. Sci., in press.

[3] Herty, M., Puppo, G., Tosin, A. and Visconti, G. 2016 *Characterisation of multivalued fundamental diagrams of traffic by Boltzmann to Fokker-Planck limit*, in preparation.

[4] Puppo, G., Semplice, M., Tosin, A. and Visconti, G. 2015 *Analysis of a heterogeneous kinetic model for traffic flow*, preprint: arXiv:1511.06395.

[5] Puppo, G., Semplice, M., Tosin, A. and Visconti, G. 2016 *Fundamental diagrams in traffic flow: the case of heterogeneous kinetic models*. Commun. Math. Sci., 14(3), 643–669.

[6] Puppo, G., Semplice, M., Tosin, A. and Visconti, G. 2016 *Kinetic models for traffic flow resulting in a reduced space of microscopic velocities*, preprint: arXiv:1507.08961.

Sub–shock formation in multi–temperature gas mixtures

Fiammetta Conforto
Università degli Studi di Messina
viale F. Stagno d'Alcontres, 31 98166 - Messina Italy
fiammetta.conforto@unime.it

The problem of sub–shock formation within a shock structure solution for hyperbolic systems of balance laws has been widely studied (see [4] and related bibliography). In [4] the authors proved non–existence of smooth solutions when the speed of propagation of the wave front exceeds the maximum eigenvalue evaluated in the unperturbed equilibrium state into which the front propagates; however, the regularity of shock structure solutions propagating with speed lower than this threshold is still an open problem.
Recently, in [3, 1, 5] shock structure solutions have been investigates in an inert binary gas mixture, described by closures at either Euler, or Grad 10–moment level of the Boltzmann equations, as well as Euler level Extended Thermodynamic models, and it was shown that the solution may exhibit up to two sub–shocks, each one relevant to the field variables characterizing one of the species, and for suitable equilibrium concentrations of the two components a sub–shock may appear even for shock speeds less than the maximum unperturbed characteristic velocity.
The aim is to investigate, both analytically and numerically, the whole hierarchy of principal sub–systems of the Grad 13–moment approximation of the kinetic equations [2] for an inert binary gas mixture, in order to determine all the different ranges of shock speeds, characterizing the different shock–structure solutions, continuous or not, and to show the existence of ranges, below the maximum unperturbed characteristic velocity, for which each constituent of the mixture may generate a jump discontinuity within the shock structure solution.

References

[1] Bisi, M., Conforto, F., Martalò, G. 2015 *Sub–shock formation in Grad 10 moment equations for a binary gas mixture*. Continuum Mech. Thermodyn. DOI 10.1007/s00161-015-0476-8.

[2] Bisi, M., Groppi, M., Spiga, G. 2002 *Grad's distribution functions in the kinetic equations for a chemical reaction*. Continuum Mech. Thermodyn. 14, 207–222.

[3] Bisi, M., Martalò, G., Spiga, G. 2014 *Shock wave structure of multi–temperature Euler equations from kinetic theory for a binary mixture*. Acta Appl. Math. 132(1), 95–105.

[4] Boillat, G., Ruggeri, T. 1998 *On the shock structure problem for hyperbolic system of balance laws and convex entropy*. Cont. Mech. Thermodyn. 10(5), 285–292.

[5] Conforto, F., Mentrelli, A., Ruggeri, T. 2016 *Shock structure and multiple sub–shocks in binary mixtures of Eulerian fluids*. Ricerche di Matematica DOI: 10.1007/s11587-016-0299-3.

Sound Propagation in Binary Gas Mixtures according to Different Kinetic Models of the Boltzmann Equation

Silvia Lorenzani
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
silvia.lorenzani@polimi.it

Sound-wave propagation through a gas is known to be adequately described by the continuum Navier-Stokes equations, provided the characteristic length of the gas flow domain is significantly larger than the molecular mean free path. In the low-frequency limit, the ordinary hydrodynamics predicts that the sound velocity will be independent of frequency and the absorption will be proportional to the frequency [8], [9]. However, if the excitation frequency ω of the sound wave becomes sufficiently high, the classical continuum approach fails even at ordinary densities, because ω^{-1} can become of the order of the molecular mean free time. In particular, the usual Navier-Stokes description leads to an infinite phase velocity as the frequency goes to infinity. Therefore, in the case of rarefied gas dynamics (or equivalently, in the case of a highly oscillatory phenomenon), there is no recourse but to turn to the kinetic theory and the Boltzmann equation [11], [3], [4], [7]. A correct description of sound propagation through a rarefied gas is very important in connection with the evaluation of damping forces in micro-electro-mechanical systems (MEMS) devices vibrating at high frequencies. In this frame, it is relevant to analyze not only the damping forces exerted by single-component gases, but also those exerted by gas mixtures, since during the wafer bonding process a mixture of noble gases (like Ar, Kr or Ne) and getterable gases (like N_2, O_2 or CO_2) is usually backfilled into the MEMS sensor package to set its operating pressure ('backfilling process'). Furthermore, a deeper analysis of forced sound propagation in a gas mixture is expected to be particularly interesting in order to clarify the long standing open question about the precise nature of the several simultaneous sound modes excited in disparate-mass gas mixtures (composed of very heavy plus very light molecules) [5], [6]. The kinetic description of a mixture of gases with different particle masses (and possibly with different internal energies) is not a trivial generalization of the classical Boltzmann theory for a single gas, since the collision operators have to take into account exchanges of momentum and energy among the different species. Therefore, since it is difficult, in general, to manage the collision integral operator as such, a large number of simplified kinetic models have been developed in the literature. Among them, the one proposed by McCormack has been, over the years, the most widely used to study a great variety of problems, since all transport coefficients (i.e. viscosity, thermal conductivity, diffusion and thermal diffusion ratio) can be correctly obtained from it applying the Chapman-Enskog procedure (and the model is suitable for general intermolecular force laws) [10]. Very recently, Bisi and Lorenzani have studied in [2] the propagation of high-frequency sound waves in binary gas mixtures flowing through microchannels by using a kinetic model of BGK-type proposed by Andries et al. in [1]. Even if the BGK-Boltzmann equation generally cannot match all the transport coefficients simultaneously, in the current work, we prove that, for the specific problem at hand,

the BGK equation is a valuable tool for investigation, giving results in close agreement with those obtained through the use of more refined kinetic models. The advantage of this simplified approach is that the equations which describe the BGK model are much simpler than those which describe, for instance, the McCormack model, allowing also a semi-analytical solution that enables us to trace the origin of the physical characteristics typical of a mixture.

References

[1] Andries, P., Aoki, K. and Perthame, B. 2002 *A consistent BGK–type model for gas mixtures.* J. Stat. Phys. 106, 993–1018.

[2] Bisi, M. and Lorenzani, S. 2016 *High-frequency sound wave propagation in binary gas mixtures flowing through microchannels.* Phys. Fluids 28, 052003-21.

[3] Cercignani, C. 1988 *The Boltzmann equation and its applications.* Springer, New York.

[4] Hadjiconstantinou, N. G. and Garcia, A. L. 2001 *Molecular simulation of sound wave propagation in simple gases.* Phys. Fluids 13, 1040–1046.

[5] Huck, R. J. and Johnson, E. A. 1980 *Possibility of double sound propagation in disparate-mass gas mixtures.* Phys. Rev. Lett. 44, 142–145.

[6] Johnson, E. A. 1989 *Two–temperature hydrodynamics and multiple sound modes in disparate–mass gas mixtures.* J. Stat. Phys. 57, 647–664.

[7] Kalempa, D. and Sharipov, F. 2009 *Sound propagation through a rarefied gas confined between source and receptor at arbitrary Knudsen number and sound frequency.* Phys. Fluids 21, 103601–14.

[8] Landau, L. D. and Lifshitz, E. M. 1989 *Fluid Mechanics.* Pergamon, New York.

[9] Lighthill, J. 1978 *Waves in Fluids.* Cambridge University Press, New York.

[10] McCormack, F. J. 1973 *Construction of linearized kinetic models for gaseous mixtures and molecular gases.* Phys. Fluids 16, 2095–2105.

[11] Sirovich, L. and Thurber, J. K. 1965 *Propagation of forced sound waves in rarefied gasdynamics.* J. Acoust. Soc. Am. 37, 329–339.

Advanced Numerical Techniques for Hyperbolic Problems

PROPOSERS

Sebastiano Boscarino
Università degli Studi di Catania
Dipartimento di Matematica e Informatica, viale A.Doria 6, 95125 - Catania Italy
boscarino@dmi.unict.it

Giovanni Russo
Università degli Studi di Catania
Dipartimento di Matematica e Informatica, viale A.Doria 6, 95125 - Catania Italy
russo@dmi.unict.it

SPEAKERS

Giacomo Dimarco
Dipartimento di Matematica e Informatica, Università di Ferrara, Italy
giacomo.dimarco@unife.it

Matteo Semplice
Dipartimento di Matematica, Università di Torino, Italy
matteo.semplice@unito.it

Enrique D. Fernández-Nieto
Department of Applied Mathemmatics, University of Seville
edofer@us.es

Sebastiano Boscarino
Dipartimento di Matematica e Informatica, Università di Catania, Italy
boscarino@dmi.unict.it

The purpose of this mini symposium is to gather researchers working on novel numerical techniques for hyperbolic problems with particular interests in the theoretical, applied, and computational aspects. Hyperbolic systems are involved in the description of many physical problems, ranging from classical applications in aerodynamics to shallow water models for the simulation of waves in lakes and rivers, from combustion problems to hydrodynamic models of semiconductors, to mention just a few examples. Specific themes that will be considered in the mini symposium concern the development of numerical schemes for all Mach number flows and construction of conservative schemes based on non conservative variables.

Implicit-explicit linear multistep methods for stiff kinetic equations

Giacomo Dimarco
Università degli Studi di Ferrara
Via Machiavelli, 30 44121 - Ferrara Italy
giacomo.dimarco@unife.it

Lorenzo Pareschi
Università degli Studi di Ferrara
via Machiavelli, 30 44121 - Ferrara Italy
lorenzo.pareschi@unife.it

We consider the development of high order asymptotic-preserving linear multistep methods for kinetic equations and related problems. The methods are first developed for BGK-like kinetic models and then extended to the case of the full Boltzmann equation. The behavior of the schemes in the Navier-Stokes regime is also studied and compatibility conditions derived. We show that, compared to IMEX Runge-Kutta methods, the IMEX multistep schemes have several advantages due to the absence of coupling conditions and to the greater computational efficiency. The latter is of paramount importance when dealing with the time discretization of multidimensional kinetic equations.

The CWENO reconstruction procedure

Matteo Semplice
Università degli Studi di Torino
via Carlo ALberto, 10 10123 - Torino Italy
matteo.semplice@unito.it

Isabella Cravero
Università degli Studi di Torino
via Carlo ALberto, 10 10123 - Torino Italy
isabella.cravero@unito.it

Gabriella Puppo
Università dell'Insubria
via Valleggio, 10 - 22100 Como Italy
gabriella.puppo@uninsubria.it

Giuseppe Visconti
Università dell'Insubria
via Valleggio, 10 - 22100 Como Italy
giuseppe.visconti@uninsubria.it

An high order finite-volume scheme puts the following strain on the reconstruction procedure: it should be able to compute accurate and non-oscillatory point values of the variables at many locations on the cell boundary, starting from the cell averages on the given cell and on its neighbours. This difficulty is increased if the scheme employs h-adaptivity (wide variety in the topology of neighbours, need to compute subcell averages in refinement), well-balancing (reconstruction points also inside the cells), error indicators that require numerical quadrature on the cell.

In such situations the WENO technique suffers from the difficulty of computing suitable sets of weights for each reconstruction point (existence, optimality, non-negativity, ...). However the CWENO construction is much more flexible since the linear weights need not satify accuracy requirements. An additional advantage is that CWENO computes the nonlinear weights for a reconstruction polynomial to be later evaluated at reconstruction points and the computation of nonlinear weights need not be repeated for each reconstruction point.

Many CWENO reconstructions have been considered in the literature, up to order 4 in two space dimensions and order 5 in one space dimension. In this talk I will focus on properly defining the "CWENO reconstruction procedure" and on the specific tools needed for the analysis of its behaviour on smooth and on discontinous data. Examples will range from the classical 1D CWENO3 [1, 2, 3], to its extensions to 2D quad-tree meshes [4] and to novel 1D CWENO reconstructions of order 5 and 7 [5].

References

[1] Levy, Puppo, Russo - *Compact central WENO schemes for multidimensional conservation laws* - SIAM J. Sci. Comput. (2000)

[2] Puppo, Semplice - *Well-balanced high order schemes on non-uniform grids and entropy residuals* - J. Sci. Comput. (2016)

[3] Cravero, Semplice - *On the accuracy of WENO and CWENO reconstructions of third order on nonuniform meshes* - J. Sci. Comput. (2016)

[4] Semplice, Coco, Russo - *Adaptive Mesh Refinement for Hyperbolic Systems based on Third-Order Compact WENO Reconstruction* - J. Sci. Comput. (2016)

[5] Cravero, Puppo, Semplice, Visconti - In preparation

Eigenvalues approximation of the two-layer shallow water system: applications with finite volume solvers

Enrique D. Fernández-Nieto
Departamento de Matemática Aplicada I, Universidad de Sevilla
E.T.S. Arquitectura. Avda, Reina Mercedes, s/n. 41012 Sevilla, Spain
edofer@us.es

Manuel J. Castro Díaz
Dpto. Análisis Matem‡tico, Fac. Ciencias, Universidad de Málaga
Campus de Teatinos S/N, 29081 M‡laga (Spain)
castro@anamat.cie.uma.es

Tomás Morales de Luna
Dpto de Matemáticas, Universidad de Córdoba
Edificio C2, Campus de Rabanales, 14071 Córdoba
Tomas.Morales@uco.es

Gladys Narbona-Reina
Departamento de Matemática Aplicada I, Universidad de Sevilla
E.T.S. Arquitectura. Avda, Reina Mercedes, s/n. 41012 Sevilla, Spain
gnarbona@us.es

In this work we focus on two-layer shallow water systems, due to the applicability of these models to the simulation of stratified geophysical flows.

First, a new approximation of the eigenvalues of the two-layer shallow water system is presented. It can be seen as an improvement of the widely used approximation proposed by Schijf and Schonfeldin in 1953 in the framework of oceanographical flows, see [4]. One of the main drawbacks of this classical approximation is that it is only valid for the case with the ratio of densities is close to 1. Then, it cannot be considered in applications such as submarine avalanches (see [2]). The proposed approximation is valid for any value of the ratio of densities and verifies some other interesting properties.

Second, we consider this new approximation of the eigenvalues of the two-layer shallow water system to improve the eficiency of IFCP method (see [3]). This is a method specially designed for two-layer shallow water systems. It does not need any spectral decomposition of the matrix of the system, such as for example Roe method. Nevertheless, it is defined in terms of the approximations of their eigenvalues.

Third, we apply this new approximation of the eigenvalues to improve the numerical treatment of the loss of hyperbolicity of two-layer systems presented in [1].

Finally, several applications are considered for stratified flows and submarine avalanches.

References

[1] M.J. Castro, E.D. Fernández-Nieto, J.M. González, C. Parés, 2011 *Numerical treatment of the loss of hyperbolicity of the two-layer shallow-water system.* Journal of

scientific computing, 48: 16–40.

[2] E.D. Fernandez-Nieto, F. Bouchut, D. Bresch, M. J. Castro Díaz, A. Mangeney, 2008. *A new Savage-Hutter type model for submarine avalanches and generated tsunami.* , J. Comp. Phys., 227: 7720–7754.

[3] E. D. Fernández-Nieto, M. J. Castro Díaz, and C. Parés, 2011. *On an intermediate field capturing Riemann solver based on a parabolic viscosity matrix for the two-layer shallow water system.* J. Sci. Comput., 48(1-3): 117–140.

[4] J.B. Schijf and J.C. Schonfeld, 1953. *Theoretical considerations on the motion of salt and fresh water, in.* Proc. Minn. Int. Hydraulics Conv., joint meeting IAHR Hydro. Div. ASCE., pages 321–333, 1953.

Semi-Implicit Asymptotic Preserving Scheme for All Mach Number Flows

Sebastiano Boscarino
Dipartimento di Matematica ed informatica
Università degli Studi di Catania
via A. Doria, 6 95125 - Catania Italy
boscarino@dmi.unict.it

The computation of compressible flows becomes more challenging when the Mach number has different orders of magnitude. When the Mach number tends to zero, compressible flow equations converge to incompressible ones, the flow speed is much less that the sound speed and the acoustic waves are much faster than material waves. Then, if the Mach number is small, the acoustic waves lead to stiffness in time and excessively large numerical viscosity. In this work we develop a high order asymptotic-preserving numerical scheme for the compressible Euler equations of gas dynamics that is stable and accurate for all Mach numbers regimes and that is able to capture the incompressible Euler limit. This scheme is based on a semi-implicit discretization which treats the acoustic part implicitly and the convective parts explicitly. We present one and two dimensional numerical results both compressible and incompressible regimes.

Keywords Gas Dynamics, All Mach number, Euler Equations.

Analysis and control of degenerate evolution equations

PROPOSERS

Piermarco Cannarsa
Università degli Studi di Roma "Tor Vergata"
Via della Ricerca Scientifica 1, 00133 - Roma Italy
cannarsa@mat.uniroma2.it

Giuseppe Floridia
Università degli Studi di Napoli Federico II
Via Cintia, Monte S. Angelo I-80126 - Napoli, Italy
giuseppe.floridia@unina.it

SPEAKERS

Fatiha Alabau-Boussouira
Institut Elie Cartan de Lorraine, Université de Lorraine
fatiha.alabau@univ-lorraine.fr

Karine Beauchard
Département de Mathématiques, École Normale Supérieure de Rennes
karine.beauchard@ens-rennes.fr

Genni Fragnelli
Dip. di Matematica, Università degli Studi di Bari
genni.fragnelli@uniba.it

Cristina Pignotti
Dip. di Ingegneria e Scienze dell'Informazione e Matematica, Università degli Studi dell'Aquila
pignotti@univaq.it

Enrico Priola
Dip. di Matematica, Università degli Studi di Torino
enrico.priola@unito.it

Piermarco Cannarsa
Dip. di Matematica, Università degli Studi di Roma "Tor Vergata"
cannarsa@mat.uniroma2.it

Control and inverse problems for degenerate PDE's arise in many applications such as cloaking (building of devices that lead to invisibility properties from observation) [3], climatology [2], and vision [4]. Such a variety of applications has given birth to challenging mathematical problems for degenerate PDE's of evolution, where degeneracy may occur either on a part of the boundary or on a submanifold of the space domain. This minisymposium aims at providing a wide overview of the main results and techniques that have recently been developed to cope with degeneracy, covering parabolic equations

which have been intensively studied in recent years as well as less undertsood models, including degenerate wave equations, delay equations, and equations with jumps and noise.

References

[1] Cannarsa, P., Martinez, P. and Vancostenoble, J. 2016 *Global Carleman estimates for degenerate parabolic operators with applications*, in, Memoirs of the AMS, vol. 239, Amer. Math. Soc., Providence, RI, 1–209.

[2] Diaz, J.-I. 1993 *Mathematical analysis of some diffusive energy balance models in climatology*, in, Mathematics, climate and environment (Madrid, 1991), RMA Res. Notes Appl. Math 27, Masson, Paris, 28–56.

[3] Greenleaf, A., Kurylev, Y. Lassas, M. and Uhlmann, G. 2009 *Cloaking devices, electromagnetic wormholes, and transformation optics.* SIAM Rev. 51, 3–33.

[4] Citti, G. and Manfredini, M. 2004 *A degenerate parabolic equation arising in image processing*, Commun. Appl. Anal. 8, 125–141.

Control and inverse problems for a class of hyperbolic systems of PDE's

Fatiha Alabau-Boussouira
Institut Elie Cartan de Lorraine
Université de Lorraine
fatiha.alabau@univ-lorraine.fr

We present some recent results on the control and inverse problems for systems of PDE's. Our main concerns in these fields are to address mathematical situations and applications for which we have only partial observations or measurements on the unknowns. The challenging questions are then to determine if in spite of these lack of observations or measurements, one can get the full desired information on the unknowns. We present several results in this direction. This work is in collaboration with Piermarco Cannarsa and Masahiro Yamamoto.

Null-Controllability Of Hypoelliptic Quadratic Differential Equations

Karine Beauchard
ENS Rennes et IRMAR, Université de Rennes 1
ENS Rennes, Avenue Robert Schumann, 35170 Bruz, FRANCE
Karine.Beauchard@ens-rennes.fr

Karel Pravda-Starov
IRMAR, Université de Rennes 1
Campus de Beaulieu, 263 Avenue du général Leclerc, CS 74205, 35042 Rennes Cedex, France
karel.pravda-starov@univ-rennes1.fr

We study the null-controllability of parabolic equations associated to a general class of hypoelliptic quadratic differential operators. Quadratic differential operators are operators defined in the Weyl quantization by complex-valued quadratic symbols. We consider in this work the class of accretive quadratic operators with zero singular spaces. These possibly degenerate non-selfadjoint differential operators are known to be hypoelliptic and to generate contraction semigroups which are smoothing in specific Gelfand-Shilov spaces for any positive time. Thanks to this regularizing effect, we prove by adapting the Lebeau-Robbiano method that parabolic equations associated to these operators are null-controllable in any positive time from control regions, for which null-controllability is classically known to hold in the case of the heat equation on the whole space. Some applications of this result are then given to the study of parabolic equations associated to hypoelliptic Ornstein-Uhlenbeck operators acting on weighted L^2 spaces with respect to invariant measures. By using the same strategy, we also establish the null-controllability in any positive time from the same control regions for parabolic equations associated to any hypoelliptic Ornstein-Uhlenbeck operator acting on the flat L^2 space extending in particular the known results for the heat equation or the Kolmogorov equation on the whole space.

On some degenerate partial differential equations

Genni Fragnelli
Università degli Studi di Bari Aldo Moro
via Orabona, 4 70125 - Bari Italy
genni.fragnelli@uniba.it

We will report on some recent results about degenerate equations with regular or non smooth coefficients. In particular, we will focus on the wellposedness of the associated Cauchy problem and on some Carleman estimates that are the crucial tool to prove an obsevability inequality, and hence null controllability.

A stability result for the wave equation with Kelvin-Voigt damping and delay feedback

Cristina Pignotti
Università degli Studi di L'Aquila
via Vetoio, loc. Coppito, 67010 - L'Aquila Italy
pignotti@univaq.it

Serge Nicaise
Université de Valenciennes et du Hainaut Cambrésis
59313 Valenciennes Cedex 9 - France
serge.nicaise@univ-valenciennes.fr

We study the wave equation with localized structural damping and boundary condition with time delay. The stability problem for the wave equation with local Kelvin-Voigt damping and null Dirichlet boundary condition has been first considered by Liu and Rao [2], without any delay term. They proved an exponential stability result under suitable conditions. On the other hand, time delay effects often appear in physical models and practical applications and it is well–known that they may induce instability phenomena in several evolution problems, which are uniformly stable in absence of delay. In particular, this is the case of wave type equations (see e.g. [1]). Then, it is important to investigate the robustness of the model with respect to (small) delays.
Under appropriate assumptions, we will show that an exponential stability result still holds ([3]). The proof is obtained by a frequency domain approach based on a well-known characterization of Huang and Prüss for the uniform stability of C_0-semigroups of contractions.

References

[1] Datko, R. 1988 *Not all feedback stabilized hyperbolic systems are robust with respect to small time delays in their feedbacks*. SIAM J. Control Optim. 26, 697–713.

[2] Liu, K., Rao, B. 2006 *Exponential stability for the wave equations with local Kelvin–Voigt damping*. Z. angew. Math. Phys. 57, 419–432.

[3] Nicaise, S., Pignotti, C. 2016 *Stability of the wave equation with localized Kelvin-Voigt damping and boundary delay feedback*. Discrete Contin. Dyn. Syst. Ser. S 9, 791–813.

Well-posedness of semilinear stochastic wave equations with Hölder continuous coefficients

Enrico Priola
Università degli Studi di Torino
Dipartimento di Matematica "Giuseppe Peano" via Carlo Alberto 10 - 10123 - Torino Italy
enrico.priola@unito.it

Federica Masiero
Dipartimento di Matematica e Applicazioni
Università di Milano Bicocca
via Cozzi 55 - 20125 - Milano Italy
federica.masiero@unimib.it

We prove that semilinear stochastic abstract wave equations, including wave and plate equations, are well-posed with an α-Hölder continuous drift coefficient, if $\alpha \in (2/3, 1)$. The uniqueness may fail for the corresponding deterministic PDE and well-posedness is restored by considering an additive pertubation of white noise type which describes an external random forcing. This shows that a kind of regularization by noise holds for the semilinear wave equation. In the proof we adopt an approach based on backward stochastic equations and use non-standard regularizing properties for the transition semigroup associated to the stochastic wave equation; these properties are based on control theoretic results.

Control cost of degenerate parabolic equations

Piermarco Cannarsa
Università degli Studi di Roma "Tor Vergata"
Via della Ricerca Scientifica 1, 00133 - Roma Italy
cannarsa@mat.uniroma2.it

Patrick Martinez
Institut de Mathématiques de Toulouse
Université Paul Sabatier Toulouse III - Toulouse France
Patrick.Martinez@math.univ-toulouse.fr

Judith Vancostenoble
Institut de Mathématiques de Toulouse
Université Paul Sabatier Toulouse III - Toulouse France
judith.vancostenoble@math.univ-toulouse.fr

The null controllability properties of degenerate parabolic operators in low space dimension, via both boundary and locally distributed controls, are fairly well understood (see [1]) and will be surveyed in this talk. Special attention will be devoted to estimates for the blow-up of the cost of control as degeneracy parameters approach the controllability threshold.

References

[1] Cannarsa, P., Martinez, P. and Vancostenoble, J. 2016 *Global Carleman estimates for degenerate parabolic operators with applications*, in, Memoirs of the AMS, vol. 239, Amer. Math. Soc., Providence, RI, 1–209.

Mathematical Methods and Models in Complex Structures - Part I

PROPOSERS

Sandra Carillo
SAPIENZA Università di Roma
Dip. S.B.A.I., Via A. Scarpa 16, 00161 Rome, Italy
sandra.carillo@sbai.uniroma1.it

Claudio Giorgi
Università degli Studi di Brescia
DICATAM, via Valotti, 9 25133 Brescia, Italy
claudio.giorgi@unibs.it

SPEAKERS

Daniele Andreucci
SAPIENZA Università di Roma
daniele.andreucci@sbai.uniroma1.it

Alessia Berti
Università Telematica "E-CAMPUS"
alessia.berti@unibs.it

Sandra Carillo
SAPIENZA Università di Roma
sandra.carillo@sbai.uniroma1.it

Davide Guidetti
Dip. Matematica, Università di Bologna
davide.guidetti@unibo.it

Maria Grazia Naso
DICATAM, Università degli Studi di Brescia
mariagrazia.naso@unibs.it

Elena Vuk
DICATAM, Università degli Studi di Brescia
elena.vuk@unibs.it

The minisymposium aims to provide an overview on current research in mathematical models arising in the study of complex structures. These problems quite often originate when the behaviour of *new materials* such as materials with memory or composite materials or composite structures is investigated. Hence, for instance, one of the problems to study concerns the coupling of different physical phenomena such as viscoelasticity and magnetic effects or, the interaction between different parts of a composite structure constructed bounding together different beams or plates.

Homogenization of a parabolic problem with alternating boundary conditions

Daniele Andreucci
Sapienza Università di Roma
via Antonio Scarpa 16, 00161 Roma Italy
daniele.andreucci@sbai.uniroma1.it

Micol Amar
Sapienza Università di Roma
via Antonio Scarpa 16, 00161 Roma Italy

Dario Bellaveglia
Sapienza Università di Roma
via Antonio Scarpa 16, 00161 Roma Italy

We consider the homogenization of a parabolic problem in a perforated domain with Robin–Neumann boundary conditions oscillating in time. Boundary conditions alternating in time appear in biological applications, for example in the modeling of ion channels, see [1]. Our approach relies upon a generalization of the unfolding technique, see e.g., [2], to the time-periodic case. To this end we show how the method of periodic unfolding can be applied to classical homogenization problem for a parabolic equation with diffusion and capacity-like coefficients in the diffusion equation oscillating both in space and time, with general independent scales.
From an analytical point of view, in the present case such oscillations must compensate the blow up of the boundary measure of the holes.
We obtain a macroscopic parabolic problem containing an extra linear term due to the absorption determined by the Robin condition; this term keeps memory of the underlying temporal and spatial microstructures.

References

[1] D. Andreucci, D. Bellaveglia. Permeability of interfaces with alternating pores in parabolic problems. Asymptotic Analysis. 79 (2012), 189–227.

[2] D. Cioranescu, A. Damlamian and G. Griso. The periodic unfolding method in homogenization. SIAM Journal on Mathematical Analysis. 40(4) (2008), 1585–1620.

A mathematical model for brine channels in sea ice

Alessia Berti
Università e-Campus
via Isimbardi, 10 22060 - Novedrate (CO) Italy
alessia.berti@unibs.it

Ivana Bochicchio
Università di Salerno,
via Giovanni Paolo II, 132 84084 - Fisciano (SA) Italy
ibochicchio@unisa.it

Mauro Fabrizio
Università di Bologna,
piazza Porta S.Donato, 5 40126 - Bologna Italy
mauro.fabrizio@unibo.it

We propose a thermodynamically consistent model to study the solidification process in sea water. When sea water freezes the dissolved salt is expelled from the domains occupied by the salt (ice is composed of only pure water) and increases the salinity of the residual liquid solution. This leads to the cryoscopic effect, namely the lowering of the freezing point of the residual solution, and to the formation of a porous ice-liquid structure run through tubular structures of more concentrated solution (brine channels). The described phenomenon is relevant in environmental sciences because it affects the marine waters of the Arctic areas [6]. Indeed, brine channels represent a habitat of different polar microorganisms which constitute the basis of the food chain in these zones. In addition, sea ice formation influences the heat transfer between ocean and atmosphere and hence the climatic properties.
From a mathematical point of view, two different, but concomitant phenomena are analyzed: the ice-water phase change and the separation between salt and (frozen) water. We introduce the salt concentration c in the liquid phase, the order parameter φ for the ice-liquid phase transition and we perform a suitable decomposition of the density of the mixture of salt, water and ice.
Following the phase field approach we assume that the solid-liquid phase transition is governed by a time dependent Ginzburg-Landau equation for first order transitions [3, 4], and the separation of salt is ruled by a Cahn-Hilliard type equation [2, 5]. More precisely, we let

$$\begin{aligned}
\rho\dot{\varphi} &= \gamma_2\nabla\cdot[\rho\nabla\varphi] - \rho\theta_T F'(\varphi) - \rho[\theta+\lambda p+\alpha(c)]G_\varphi(c,\varphi),\\
\rho\dot{c} &= \nabla\cdot[M(c)\nabla\mu],\\
\mu &= -\frac{\gamma_1}{\rho}\nabla\cdot[\rho\nabla c] + \alpha'(c)G(c,\varphi) + [\theta+\lambda p+\alpha(c)]G_c(c,\varphi) + \theta_c K'(c) + \theta H'(c),
\end{aligned}$$

where ρ, θ, p represent the density of the mixture, the absolute temperature and the pressure; $F(\varphi), G(c,\varphi), K(c), H(c)$ are suitable potentials characterizing the transition and the separation; $\gamma_1, \gamma_2, \theta_T, \theta_c$ are positive constants. In addition, we suppose that the

functions $\alpha(c), M(c)$ satisfy the conditions

$$M(c) \geq 0, \quad M(0) = M(1) = 0,$$
$$\alpha(0) = 0, \quad \alpha'(c) \geq 0, \quad \alpha'(c) = 0 \ \text{ for all } c \notin (0,1)\,.$$

Since thermal and mechanical effects are relevant during phase transitions and separations, we include also into the model a heat equation for the temperature change, which is deduced by the first law of Thermodynamics, and a suitable Navier–Stokes equation. The coupling between the Navier–Stokes equation and the other involved equations is due to the presence of the material time derivative and to the Korteweg stresses proportional to $\nabla\varphi \otimes \nabla\varphi$ and $\nabla c \otimes \nabla c$.
We prove that the resulting differential model is compatible with the second law of Thermodynamics expressed by the Clausius Duhem inequality (see [1]).
Finally, we show that both c and φ remain confined within the interval $[0, 1]$ during their evolution. The mathematical difficulties in proving the maximum theorem lie in the fact that a system of equations is involved and that the spatial operator entering the governing equation of c is of fourth order. For this reason, we take two additional assumptions on the mobility, that are

(H1) $M(c) \geq 0$, $M(0) = M(1) = 0$, $\nabla M(0) = \nabla M(1) = 0$,

(H2) $M(c)\nabla\mu \cdot \nabla\mu + \gamma_1 \rho \nabla c \cdot \mathbf{D}\nabla c \geq 0$,

where $\mathbf{D}$ is the symmetrical part of the gradient of velocity [1, 5].
No assumption is placed on the phase field φ. The hypothesis (H1) ensures that $\dot{c}$ vanishes at $c = 0$, $c = 1$. A possible choice is $M(c) = M_0 c^2(1-c)^2$ with $M_0 > 0$. The second condition means that if $\mathbf{D}$ is negative definite, then it is not too large relative to the first term.

References

[1] Berti A., Bocchichio I. and Fabrizio M. 2016, *Transition and separation process in brine channels formation*, J. Math. Phys. 57, 023513.

[2] Cahn J.W. and Hilliard J.E. 1958, *Free energy of a non-uniform system. I. Interfacial free energy*, J. Chem. Phys. 28, 258–267.

[3] Fabrizio M. 2006, *Ginzburg–Landau equations and first and second order phase transitions*, Int. J. Engn. Sc. 44, 529–539.

[4] Fabrizio M. 2008, *Ice-water and liquid-vapor phase transitions by a Ginzburg-Landau model*, J. Math. Phys. 49, 102902.

[5] Fabrizio M., Giorgi C. and Morro A. 2011, *Phase separation in quasi-incompressible Cahn-Hilliard fluids*, Eur. J. Mech. 30, 281–287.

[6] Kutschan B., Morawetz K. and Gemming S. 2010, *Modeling the morphogenesis of brine channels in sea ice*, Phys. Rev. E 81, 036106 .

New Non Abelian Bäcklund Charts

Sandra Carillo
Dipartimento "Scienze di Base e Applicate per l'Ingegneria"
Sapienza - Università di Roma, 16, Via A. Scarpa, 00161 Rome, Italy
I.N.F.N. - Sez. Roma1, Gr. IV - Mathematical Methods in NonLinear Physics, Rome, Italy
sandra.carillo\char64\relaxsbai.uniroma1.it

Mauro Lo Schiavo
Dipartimento "Scienze di Base e Applicate per l'Ingegneria"
Sapienza - Università di Roma, 16, Via A. Scarpa, 00161 Rome, Italy
mauro.loschiavo\char64\relaxsbai.uniroma1.it

Cornelia Schiebold
Department of Science Education and Mathematics
Mid Sweden University, S-851 70 Sundsvall, Sweden
Instytut Matematyki, Uniwersytet Jana Kochanowskiego w Kielcach, Poland
Cornelia.Schiebold\char64\relaxmiun.se

The term Bäcklund Chart is used to denote a net of links represented by Bäcklund Transformations relating different nonlinear evolution equations. Here non-Abelian evolution equations wherein the unknown is an aperator on a Banach space are considered. The new Bäcklund Chart [3] connecting various third order non-Abelian evolution equations is presented and discussed. One of the novelties of this Bäcklund Chart is that it connects new equations: the non-Abelian counterparts of the *Korteweg deVries singuarity manifold* (KdV Sing.) [11] and of the *Korteweg deVries interacting soliton* (Int. So KdV) [8]. New are also the recursion of operators of the KdV Sing. as well as of the Int. So KdV equation. All the operators admitted by the non-Abelian evolution equations which appear in the Bäcklund Chart are proved to be hereditary. Hence, the Bäcklund Chart itself extends from the equations to the corresponding hierarchies. The Bäcklund Chart obtained in this non-Abelian operator setting represents a generalization of the analog one constructed in [9]. Furthermore, the new non-Abelian Bäcklund Chart in [3] extends that one given in [2] which allowed, [1] to construct explicit solutions of matrix Korteweg-de Vries and modified Korteweg-de Vries hierarchies.
Oberve that, the well known connection, via the cole-Hopf transformation [7, 10], between the Burgers equation and the linear heat equation can be extended to the case of the analog non-Abelian operator equations [6, 5]. Thus, in [5] the non-Abelian operator Burgers equation is proved to admit a hereditary recursion operator and the corresponding hierarchy is constructed. Different non-Abelian operator Burgers equation and hierarachies are studied in [4]. Finally, perspective work and open problems are discussed.

References

[1] S. Carillo and C. Schiebold. Matrix Korteweg-de Vries and modified Korteweg-de Vries hierarchies: Non-commutative soliton solutions. *J. Math. Phys.* **52**, 053507, (2011).

[2] S. Carillo and C. Schiebold, Non-commutative KdV and mKdV hierarchies via recursion methods. *J. Math. Phys.* **50**, 073510, (2009).

[3] S. Carillo, M. Lo Schiavo and C. Schiebold, (*arxiv.org* 1512.02386v1) submitted (2015).

[4] S. Carillo, M. Lo Schiavo and C. Schiebold, submitted (2016).

[5] S. Carillo and C. Schiebold On the recursion operator for the non-commutative Burgers hierarchy, *J. Nonlinear Math. Phys.*, **19** n.ro 1 (2012).

[6] S. Carillo and C. Schiebold *A non-commutative operator-hierarchy of Burgers equations and Bäcklund transformations*, in *Applied and Industrial Mathematics in Italy III: Selected Contributions from the 9th SIMAI Conference*, E. De Bernardis, R. Spigler e V. Valente Ed.s, SERIES ON ADVANCES IN MATHEMATICS FOR APPLIED SCIENCES, vol.82, 175 –185, World Scientific Pubbl., Singapore, (2009).

[7] J.D. Cole On a quasilinear parabolic equation occuring in aerodynamics *Quart.App. Math.***92**, 25-236, (1951).

[8] B. Fuchssteiner. Solitons in interaction. *Progr. Theor. Phys.***78**, no. 5, 1022-1050, (1987).

[9] B. Fuchssteiner and S. Carillo, Soliton structure versus singularity analysis:third order completely integrable non linear differential equations in $1+1$-dimensions, *Physica A*, **154**, 467-510, (1989).

[10] E. Hopf The partial differential equation $u_t + uu_x = muu_{xx}$. *Comm. Pure Appl. Math.* **3**, 201–230, (1950).

[11] J. Weiss, M. Tabor and G. Carnevale, The Painlevé property for partial differential equations, *J. Math. Phys.* **24**, 522-526, (1983).

On linear parabolic mixed problems with dynamic and Wentzell boundary conditions

Davide Guidetti
Università degli Studi di Bologna
via Zamboni, 33 40126 - Bologna Italy
davide.guidetti@unibo.it

Linear parabolic problems with dynamic and Wentzell boundary conditions have been object of intensive research in these latest years (see the bibliographies in [1] and [2]). They appear in applications connected with heat transfer problems in a solid in contact with a fluid, in neurological problems and diffusion on networks (see [3], [4], [5]). We present some results of maximal regularity in L^p spaces and spaces of Hölder continuous functions.

References

[1] Guidetti D., 2014 *Abstract elliptic problems depending on a parameter and parabolic problems with dynamic boundary conditions*, Springer Indam Series 10, 161–202.

[2] Guidetti D., 2016 *Linear parabolic problems with dynamic boundary conditions in spaces of Hölder continuous functions*, Ann. Mat. Pura Appl. 195, 167–198.

[3] Hömberg D., Krumbiegel K., Rehberg J., 2013 *Optimal control of a parabolic equation with dynamic boundary conditions*, Appl. Math. Optim. 67 (2013), 3–31.

[4] Langer R.E., 1932 *A problem in diffusion or in the flow of heat for a solid in contact with a fluid*, Tohoku Math. Journ. 35, 260–275.

[5] Ruiz Goldstein G., 2006 *Derivation and physical interpretation of general boundary conditions*, Adv. Diff. Eq. 11, 457–480.

How to stabilize a Timoshenko system?

Maria Grazia Naso
Università degli Studi di Brescia
Via Valotti 9, 25133 - Brescia Italy
mariagrazia.naso@unibs.it

In 1921 S. Timoshenko proposed a coupled hyperbolic system describing the transverse vibration of a beam, but without the presence of any damping. Therefore that system is conservative, and so the related total energy of the beam remains constant along the time. The subject of stability of Timoshenko-type systems has been a research topic that has attracted considerable interest and a lot of attention in the last years. Quite a number of results concerning uniform and asymptotic decay of energy have been established. An important issue of research is to look for a minimum dissipation by which solutions of system decay uniformly to zero as time goes to infinity. In this regard, several types of dissipative mechanisms have been introduced, such as dissipative mechanism of frictional type, of viscoelastic type and thermal dissipation. In this talk, we will analyze the decay rate of the energy of the Timoshenko beam with one boundary dissipation acting in the rotation-angle equation.

A vector-valued model for the Curie transition in ferroelectrics

Elena Vuk
Università degli Studi di Brescia
via D. Valotti, 9 25133 - Brescia Italy
elena.vuk@unibs.it

Alessia Berti
Università E-Campus
via Isimbardi, 10 22060 - Novedrate (CO) Italy
alessia.berti@unibs.it

Claudio Giorgi
Università degli Studi di Brescia
via D. Valotti, 9 25133 - Brescia Italy
claudio.giorgi@unibs.it

Ferroelectricity is a property of certain materials that have a spontaneous electric polarization that can be reversed by the application of an external electric field. The distinguishing feature of ferroelectrics is that the spontaneous polarization can be reversed by a suitably strong applied electric field in the opposite direction; the polarization is therefore dependent not only on the current electric field but also on its history, yielding a hysteresis loop. Typically, such materials demonstrate ferroelectricity only below a certain phase transition temperature, called the Curie temperature, θ_C. Above this temperature the spontaneous polarization vanishes, and the ferroelectric crystal transforms into the paraelectric state. These materials are called *ferroelectrics* by analogy to ferromagnetic materials, which exhibit spontaneous magnetization and similar hysteresis loops [1].

According to [4], we assume that there exists a suitable constitutive function $\boldsymbol{\mathcal{P}}$ such that the evolution of the polarization vector $\boldsymbol{P}$ is ruled by means of a constitutive equation of the rate type

$$\dot{\boldsymbol{P}} = \boldsymbol{\mathcal{P}}(\theta, \boldsymbol{P}, \boldsymbol{\mathcal{E}}),$$

where $\boldsymbol{\mathcal{E}}$ represents the *effective electric field* acting inside the matter. This field differs from the external electric field $\boldsymbol{E}$ by the sum of several contributions due, for instance, to anisotropy, exchange interactions and the interaction of the polarization field with itself.

Borrowing from the Landau-Lifschitz-Bloch equation for ferromagnets [2], we propose the following explicit kinetic equation ruling the evolution of the polarization vector both at high and low temperatures,

$$\boldsymbol{\mathcal{P}} = -\frac{\gamma}{P}\,\boldsymbol{P}\times\boldsymbol{\mathcal{E}} - \frac{\beta}{P^2}\,\boldsymbol{P}\times(\boldsymbol{P}\times\boldsymbol{\mathcal{E}}) + \frac{\alpha}{P^2}\,(\boldsymbol{\mathcal{E}}\cdot\boldsymbol{P})\,\boldsymbol{P}, \tag{1}$$

where P stands for the modulus of $\boldsymbol{P}$, while α, β and γ are suitable coefficients depending on θ, only. Assuming that all interactions inside the matter depend on a thermodynamic potential and letting $\hat{\psi} = \psi/\theta$ the rescaled Helmholtz free energy, we denote

$$\boldsymbol{\mathcal{E}} = \boldsymbol{E} - \frac{1}{\epsilon_0}\delta_{\mathbf{P}}\hat{\psi}, \tag{2}$$

where ϵ_0 is the vacuum dielectric constant and $\delta_{\boldsymbol{P}}$ denotes the variational derivative with respect to the field $\boldsymbol{P}$, namely $\delta_{\boldsymbol{P}}\hat{\psi} = \partial_{\boldsymbol{P}}\hat{\psi} - \nabla \cdot \partial_{\nabla \boldsymbol{P}}\hat{\psi}$. Starting from a suitable choice of the free energy which accounts for the physical assumptions in ferroeletric media, the explicit form of $\boldsymbol{\mathcal{E}}$ is obtained.
From thermodynamic arguments we reach the *dissipation condition*

$$\boldsymbol{\mathcal{E}} \cdot \boldsymbol{\mathcal{P}} \geq 0, \tag{3}$$

and we prove that it is fulfilled by (1) provided that $\alpha, \beta \geq 0$.
Finally, we discuss two suitable choices of the Gibbs free energy which are usually referred to as *Landau free energy* and *Langevin free energy*. Then, by exploiting the Ginzburg-Landau theory of phase transitions in a neighborhood of the Curie temperature [3], we are able to describe the phase transition between the paraelectric and ferroelectric regimes.

References

[1] Damjanovic, D. 2005 Hysteresis in Piezoelectric and Ferroelectric Materials. In *The Science of Hysteresis* (ed. I. Mayergoyz and G. Bertotti), vol.3, pp. 337–465. Elsevier.

[2] Berti, A. and Giorgi, C. 2016 *Derivation of the Landau-Lifshitz-Bloch equation from continuum thermodynamics* (submitted to *Physica B*)

[3] Landau, L.D., Lifshitz, E.M. and Pitaevskii, L.P. 1984 *Electrodynamics of Continuous Media.* Oxford.

[4] Morro, A. 2007 *A phase-field model for the paraelectric-ferroelectric transition.* Appl. Math. Sci. 1, 2939–2953.

Mathematical Methods and Models in Complex Structures - Part II

PROPOSERS

Sandra Carillo
SAPIENZA Università di Roma
Dip. S.B.A.I., Via A. Scarpa 16, 00161 Rome, Italy
sandra.carillo@sbai.uniroma1.it

Claudio Giorgi
Università degli Studi di Brescia
DICATAM, via Valotti, 9 25133 Brescia, Italy
claudio.giorgi@unibs.it

SPEAKERS

Cecilia Cavaterra
Università degli Studi di Milano
cecilia.cavaterra@unimi.it

Monica Conti
(to be confirmed) Politecnico di Milano
monica.conti@polimi.it

Luciano Pandolfi
Politecnico di Torino,
luciano.pandolfi@polito.it

Maurizio Romeo
Università degli Studi di Genova
maurizio.romeo@unige.it

Vincenzo Tibullo
(to be confirmed) Università degli Studi di Salerno
vtibullo@unisa.it

Filippo Dell'Oro
Politecnico di Milano
filippo.delloro@polimi.it

The minisymposium aims to provide an overview on current research in mathematical models arising in the study of complex structures. These problems quite often originate when the behaviour of *new materials* such as materials with memory or composite materials or composite structures is investigated. Hence, for instance, one of the problems to study concerns the coupling of different physical phenomena such as viscoelasticity and magnetic effects or, the interaction between different parts of a composite structure constructed bounding together different beams or plates.

Global strong solutions of the full Navier-Stokes and Q-tensor system in 2D: existence and long-time behavior

Cecilia Cavaterra
Dipartimento di Matematica, Università degli Studi di Milano
via Cesare Saldini, 50 20133 - Milano Italy
cecilia.cavaterra@unimi.it

Elisabetta Rocca
Dipartimento di Matematica, Università degli Studi di Pavia
via Ferrata, 5 27100 - Pavia Italy
elisabetta.rocca@unipv.it

Hao Wu
School of Mathematical Sciences, Fudan University
200433 - Shanghai China
haowufd@yahoo.com

Xiang Xu
Department of Mathematics and Statistics, Old Dominion University
23529 - Norfolk, VA USA
x2xu@odu.edu

We consider a full Navier-Stokes and Q-tensor system for incompressible liquid crystal flows of nematic type. In the two dimensional periodic case, we prove the existence and uniqueness of global strong solutions that are uniformly bounded in time. This result is obtained without any smallness assumption on the physical parameter ξ that measures the ratio between tumbling and aligning effects of a shear flow exerting over the liquid crystal directors. Moreover, we show the uniqueness of asymptotic limit for each global strong solution as time goes to infinity and provide an uniform estimate on the convergence rate.

Attractors for processes on time-dependent spaces

Monica Conti
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
monica.conti@polimi.it

Vittorino Pata
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
vittorino.pata@polimi.it

The evolution of systems arising from mechanics and physics is described in many instances by differential equations of the form

$$u_t = A(u,t), \qquad u(\tau) = u_\tau \in X,$$

where X is a normed space and, for every fixed $t > \tau$, $A(\cdot, t)$ is a suitable operator on X. Assuming the Cauchy problem is well posed and calling $u(t)$ the solution at time t, the family of solving operators

$$U(t,\tau) : X \to X \quad t \geq \tau,$$

defined by

$$U(t,\tau)u_\tau = u(t)$$

is called a *process*. The issue of understanding the longtime behavior of solutions to dynamical systems is thus translated into studying the dissipative properties of the operators $U(t,\tau)$. A well-established theory of attractors provides nowadays a full description of many important autonomous systems from mathematical physics, including nonautonomous models with time-dependent external forces. In this talk we present a recent theory of attractors on time-dependent spaces, namely

$$U(t,\tau) : X_\tau \to X_t \quad t \geq \tau,$$

where the normed spaces X_t are allowed to vary at different times t. The goal is to provide an efficient tool to describe the regime behavior of evolution problems where the coefficients of the differential operator depend explicitly on time, leading to time-dependent terms at a functional level. We also discuss some possible applications of the new theory.

Control properties of Viscoelastic plates with large memory

Luciano Pandolfi
Dipartimento di Scienze Matematiche
Politecnico di Torino
luciano.pandolfi@polito.it

A viscoelastic plate (viscoelasticity of the Maxwell-Boltzmann type) is described by a Volterra integrodifferential equation

$$w'' = \Delta^2 w + \int_0^t M(t-s)\Delta^2 w(s)\,\mathrm{d}s \qquad (\mathbf{A})$$

where $M(t)$ is a memory kernel with suitable properties. Here $w = w(x,t)$ with $t > 0$ and $x \in \Omega \subseteq \mathbb{R}^2$ (a suitable region whose boundary we assume smooth). Equation **(A)** has to be supplemented with initial conditions (in a suitable *state space*) and Δ is the laplace operator. We consider the case that a control f acts on the plate via the boundary conditions:

$$\begin{cases} \text{either } \textbf{case (A)}: & \gamma_0 w = g\,,\ \gamma_1 w = 0 \\ \text{or } \textbf{case (B)}: & \gamma_0 w = 0\,,\ \gamma_1 w = g \end{cases}$$

(here γ_0 denotes the trace on the boundary, and γ_1 denotes the normal derivative). Controllability is known to hold when $M(t) \equiv 0$, i.e. for the case of a purely elastic plate, in suitable spaces. A noticeable fact is that controllability holds at every time $T > 0$.
Here we show that the same controllability properties is inherited by the viscoelastic plate, for every (smooth) memory kernel $M(t)$ and every time $T > 0$, precisely in the same spaces.
The proof combines operator methods and the properties of suitable Riesz sequences of functions, specifically related to the equation of the viscoelastic plate.

Microcontinuum model of electromagneto-elastic media and application to surface waves

Maurizio Romeo
DIMA, Università degli Studi di Genova
via Dodecaneso 35, 16146 - Genova Italy
maurizio.romeo@unige.it

In current macroscopic theories, physical interactions due to electromagnetic field in matter are modeled on the basis of Maxwell's equations, balance laws and suitable constitutive equations, compatible with thermodynamics, accounting for specific material properties. Along this line, comprehensive phenomenological continuum theories were established (see for example [3]). Microscopic models of lattice structures have supported these theories and at the same time, have legitimated the emergent investigations on continua with microstructure [1]. The classic micromorphic theory of electromagnetic interactions, beside the introduction of pertinent couplings into the balance equations, accounts for polarization and magnetization via constitutive functions of macro and micro-strain measures and of the electromagnetic field [1, 2]. As a consequence, the phenomenological model includes an increased number of unknown material parameters. An alternative micromorphic approach has been recently proposed where polarization and magnetization are introduced on the basis of the charge distribution within the continuum micro-element [5].
Here we resume the basic elements of this self-consistent physical approach and give some fundamental results. Firstly we show that electric multipoles are connected to macro and micro deformation via suitable evolution equations. Secondly, we exploit these equations to derive the macroscopic form of Maxwell's equations obtaining, as a direct consequence, the pertinent expression for polarization and magnetization. Then, in view of applications to definite problems, we reduce the general model to the micropolar one and apply it to the propagation of surface waves. Both Rayleigh and Bleustein-Gulyaev waves are considered for an hexagonal dielectric material. We compare the dispersion equations and the depth dependence of fields with those obtained in the past by phenomenological theories [4].

References

[1] Eringen, A.C. 1999 *Microcontinuum Field Theories I-Foundations and Solids*, Springer Verlag, New York.

[2] Lee, J.D, Chen, Y., Eskandarian, A. 2004 *A micromorphic electromagnetic theory.* Int. J. Solids Struct. 41, 2099-2110.

[3] Maugin, G.A. 1988 *Continuum Mechanics of Electromagnetic Solids*, North Holland, Amsterdam.

[4] Pouget, J., Maugin, G.A. 1981 *Bleustein-Gulyaev surface modes in elastic ferroelectrics*. J. Acoust. Soc. Am. 69, 1304-1318. *Piezoelectric Rayleigh waves in elastic ferroelectrics*. J. Acoust. Soc. Am. 69, 1319-1325.

[5] Romeo, M. 2011 *Micromorphic continuum model of electromagnetoelastic solids*. J. Appl. Math. Phys. (ZAMP) 62, 513-527.

On the time differential dual-phase-lag heat conduction

Vincenzo Tibullo
Università degli Studi di Salerno
via Giovanni Paolo II, 132 84084 - Fisciano Italy
vtibullo@unisa.it

Stan Chiriţă
Octav Mayer Institute of Mathematics, Romanian Academy, Iaşi Branch
Bd. Carol I, 8 700505 - Iaşi Romania
schirita@uaic.ro

Michele Ciarletta
Università degli Studi di Salerno
via Giovanni Paolo II, 132 84084 - Fisciano Italy
mciarletta@unisa.it

In this paper we study the dual-phase-lag model of heat conduction incorporating the microstructural interaction effects in the fast-transient process of heat transport. Tzou [1, 2, 3] (see also [4] and [5] and the references therein) proposed the following time differential constitutive law for the heat flux vector q_i

$$\begin{aligned} &q_i(\mathbf{x},t)+\tau_q\frac{\partial q_i}{\partial t}(\mathbf{x},t)+\frac{1}{2}\tau_q^2\frac{\partial^2 q_i}{\partial t^2}(\mathbf{x},t)\\ &=-k_{ij}(\mathbf{x})T_{,j}(\mathbf{x},t)-\tau_T k_{ij}(\mathbf{x})\frac{\partial T_{,j}}{\partial t}(\mathbf{x},t)\,, \end{aligned} \tag{1}$$

where $\tau_q \geq 0$ and $\tau_T \geq 0$ are the delay times, T is the temperature variation and k_{ij} is the conductivity tensor. It was established by Fabrizio and Lazzari [6] that the restrictions imposed by thermodynamics on the constitutive equation (1), within the framework of a linear rigid conductor, implies that the delay times have to satisfy the inequality $0 \leq \tau_q \leq 2\tau_T$.
When the constitutive equation (1) is coupled with the energy equation

$$-q_{i,i}+\varrho r=a\frac{\partial T}{\partial t}, \tag{2}$$

and under appropriate regularity assumptions, then we obtain the following governing equation of hyperbolic type for temperature field T

$$\begin{aligned} &\left(1+\tau_q\frac{\partial}{\partial t}+\frac{1}{2}\tau_q^2\frac{\partial^2}{\partial t^2}\right)\left(a\frac{\partial T}{\partial t}-\varrho r\right)\\ &=\left[k_{ij}\left(1+\tau_T\frac{\partial}{\partial t}\right)T_{,j}\right]_{,i}. \end{aligned} \tag{3}$$

Such equation was studied intensively in literature in many papers. Quintanilla [10] has shown that the equation (3), together with suitable initial conditions for T, $\frac{\partial T}{\partial t}$ and $\frac{\partial^2 T}{\partial t^2}$ and appropriate boundary conditions in terms of T, leads to an exponentially stable system when $0 < \tau_q < 2\tau_T$ and to an unstable system when $0 < 2\tau_T < \tau_q$. While in [7, 8, 9] the well-posedness problem is studied, provided some appropriate restrictions upon the parameters τ_q and τ_T are assumed. We have to outline that a second-order approximation of the Tzou's theory was studied recently by Amendola *et al.* [11].
In [12] the authors investigate the propagation of plane time harmonic waves and surface waves in the case of a homogeneous and isotropic thermoelastic material.
In the present paper we formulate the initial boundary value problem of heat conduction model based on the constitutive equation (1) and the basic energy equation (2), considering it is described by a differential system for the unknown couple $\{T, q_i\}$. That means we consider initial conditions for T, q_i and $\frac{\partial q_i}{\partial t}$ and appropriate boundary conditions in terms of temperature variation and heat flux vector. Then we study the uniqueness and continuous data dependence results as well as the spatial behavior of transient solutions and of the harmonic vibrations. The uniqueness results are established without any restrictions upon the delay times. However, there is an open problem for the class of materials characterized by zero delay time of phase lag of the conductive temperature gradient and for which the delay time in the phase lag of heat flux vector is strictly positive. In such a case it should be expected to have an ill-posed model. Moreover, it was shown by Fabrizio and Lazzari [6] that the corresponding model (with $\tau_T = 0$ and $\tau_q > 0$) is incompatible with the thermodynamic principles.
We also address the problem of continuous dependence of solutions with respect to the given data. To this aim we establish appropriate conservation laws and then we use the Gronwall's inequality in order to establish two estimates describing the continuous dependence of solutions with respect to the prescribed initial data and with respect to the given supply terms. The first estimate is established for delay times satisfying the inequality $0 \leq \tau_q \leq 2\tau_T$, which is in accord with the thermodynamic restriction established by Fabrizio and Lazzari [6]. The second estimate is established under the assumption $0 < \tau_T < \frac{\tau_q}{2}$ and it allows the solutions to have a growth exponential in time.
Finally we proceed to study the spatial behavior of transient solutions and to this end we establish a domain of influence theorem, provided the delay times satisfy $0 < \tau_q \leq 2\tau_T$. When the delay times satisfy $0 < \tau_T < \frac{1}{2}\tau_q$ we are able to establish, in the time interval $\left(0, \frac{1}{2\sigma^2}\right)$, $\sigma^2 = \frac{1}{\tau_T} - \frac{2}{\tau_q}$, an estimate of Saint-Venant type. Moreover, for the steady-state vibrations we establish an exponential decaying estimate in terms of the amplitude vibration, provided the frequency is lower than a critical value and for delay times $\tau_q \geq 0$ and $\tau_T \geq 0$.

References

[1] D. Y. Tzou, A unified approach for heat conduction from macro to micro-scales. Journal of Heat Transfer 117 (1995) 8–16

[2] D. Y. Tzou, The generalized lagging response in small-scale and high-rate heating. International Journal of Heat and Mass Transfer 38 (1995) 3231–3234

[3] D. Y. Tzou, Experimental support for the lagging behavior in heat propagation. Journal of Thermophysics and Heat Transfer 9 (1995) 686–693

[4] D. Y. Tzou, Macro- To Micro-Scale Heat Transfer: The Lagging Behavior. John Wiley & Sons, Chichester, 2015

[5] D. S. Chandrasekharaiah, Hyperbolic thermoelasticity: A review of recent literature. Applied Mechanics Reviews 51(1998) 705–729

[6] M. Fabrizio, B. Lazzari, Stability and second law of thermodynamics in dual-phase-lag heat conduction. International Journal of Heat and Mass Transfer 74 (2014) 484–489

[7] L. Wang, M. Xu, X. Zhou, Well-posedness and solution structure of dual-phase-lagging heat conduction. International Journal of Heat and Mass Transfer 44 (2001) 1659–1669

[8] L. Wang, M. Xu, Well-posedness of dual-phase-lagging heat equation: higher dimensions. International Journal of Heat and Mass Transfer 45 (2002) 1165–1171

[9] M. Xu, L. Wang, Thermal oscillation and resonance in dual-phase-lagging heat conduction. International Journal of Heat and Mass Transfer 45 (2002) 1055–1061

[10] R. Quintanilla, Exponential stability in the dual-phase-lag heat conduction theory. Journal of Non-Equilibrium Thermodynamics 27 (2002) 217–227

[11] G. Amendola, M. Fabrizio, M. Golden, B. Lazzari, Second-order approximation for heat conduction: Dissipation principle and free energies. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 472 (2016) art. no. 20150707.

[12] S. Chiriţă, M. Ciarletta, V. Tibullo, On the wave propagation in the time differential dual-phase-lag thermoelastic model. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 471 (2015), art. no. 20150400.

Elastically-coupled double-beam systems: analysis of the steady states

Filippo Dell'Oro
Politecnico di Milano
Via Bonardi 9, 20133 Milano, Italy
filippo.delloro@polimi.it

Claudio Giorgi
Università degli Studi di Brescia - DICATAM
Via Valotti 9, 25133 Brescia, Italy
claudio.giorgi@unibs.it

Vittorino Pata
Politecnico di Milano
Via Bonardi 9, 20133 Milano, Italy
vittorino.pata@polimi.it

Given $\beta \in \mathbb{R}$ and $\varrho, k > 0$, we analyze an abstract version of the nonlinear stationary model in dimensionless form

$$\begin{cases} u'''' - \Big(\beta + \varrho \int_0^1 |u'(s)|^2 \, \mathrm{d}s\Big) u'' + k(u - v) = 0 \\ v'''' - \Big(\beta + \varrho \int_0^1 |v'(s)|^2 \, \mathrm{d}s\Big) v'' - k(u - v) = 0 \end{cases}$$

describing the equilibria of an elastically-coupled extensible double-beam system subject to evenly compressive axial loads. Necessary and sufficient conditions in order to have nontrivial solutions are established, and their explicit closed-form expressions are found. In particular, the solutions are shown to exhibit at most three nonvanishing Fourier modes. In spite of the symmetry of the system, nonsymmetric solutions appear, as well as solutions for which the elastic energy fails to be evenly distributed. Such a feature turns out to be of some relevance in the analysis of the longterm dynamics, for it may lead up to nonsymmetric energy exchanges between the two beams, mimicking the transition from vertical to torsional oscillations.

Numerical Methods for Optimal Control Problems and Differential Games

PROPOSERS

Elisabetta Carlini
"Sapienza" Università di Roma
P.le Aldo Moro, 5 00185 - Roma Italy
carlini@mat.uniroma1.it

Roberto Ferretti
Università Roma Tre
L.go S. Leonardo Murialdo, 1 00146 - Roma Italy
ferretti@mat.uniroma3.it

SPEAKERS

Simone Cacace
Dip. di Matematica, "Sapienza" Università di Roma
cacace@mat.uniroma1.it

Adriano Festa
RICAM - Johann Radon Institute for Computational and Applied Mathematics
adriano.festa@oeaw.ac.at

Nicolas Forcadel
Laboratoire de Mathématiques, INSA-Rouen
nicolas.forcadel@insa-rouen.fr

Athena Picarelli
Mathematical Institute, University of Oxford
picarelli@maths.ox.ac.uk

Marie-Therese Wolfram
University of Warwick
m.wolfram@warwick.ac.uk

Hasnaa Zidani
Unité de Mathématique Appliquée, ENSTA–Paristech
housnaa.zidani@ensta-paristech.fr

Optimal control is a branch of control theory devoted to the construction of control strategies optimizing some given performance index in the operation of a controlled system described by Ordinary or Partial Differential Equations. In addition to the classical fields of application (e.g., robotics, spacecraft control, decision theory), extensions of this theory also appear in the treatment of two-player games and multi-agent systems.

The minisymposium is conceived to provide an outline of some recent directions of research in the field of optimal control, differential games and related problems. Within this scope, the main focus will be on dynamic programming (DP) techniques. In fact,

despite their computational complexity, numerical DP techniques have undergone a great development in the last decades, and are gaining an increasing interest in the optimal control community. The lines of research involved in the minisymposium include, but are not limited to, stochastic optimal control, flow on networks, hybrid control systems and mean field games.

An efficient numerical method for Stationary Mean Field Games

Simone Cacace
Dipartimento di Matematica, Sapienza Università di Roma
Piazzale Aldo Moro, 5 00185 - Roma Italy
cacace@mat.uniroma1.it

Fabio Camilli
Dipartimento di Scienze di Base e Applicate per l'Ingegneria, Sapienza Università di Roma
Via Antonio Scarpa, 16 00161 - Roma Italy
camilli@dmmm.uniroma1.it

Mean Field Games (MFG) theory has been introduced by J.M. Lasry and P.L. Lions in [3], in order to study differential games in which the number of players goes to infinity. The limit behavior of the underlying optimal control problem is then described by a system of nonlinear PDEs, namely a Hamilton-Jacobi-Bellman equation coupled with a Fokker-Planck equation. The first equation provides an optimal control for each player, according to the mass distribution of all the players, whereas the second equation evolves the mass distribution employing the optimal strategy of each player.
The theory is very flexible to many applicative fields and is attracting an ever increasing interest with several applications in economics, physics and biology. In this respect, the long time behavior of the MFG system is of particular interest, since it provides Nash equilibria for the associated differential game. This leads to solve stationary MFG systems of ergodic type, increasingly demanding for the development of efficient numerical methods.
In this talk we present a new approach to the numerical solution of Stationary Mean Field Games (see [1], [2]). It is based on a Newton-like method for inconsistent systems of nonlinear equations, arising in the discretization of the corresponding Ergodic Hamilton-Jacobi-Bellman and Fokker-Planck equations. We avoid completely classical approaches based on regularization techniques, such as ergodic and long time approximations, solving the stationary MFG system directly. We show that the new method is able to solve efficiently MFG systems on Euclidean spaces and Networks, also in the case of more competing populations and for homogenization problems. We present several numerical experiments in dimension one and two, showing the performance of the proposed method in terms of accuracy, convergence and computational time.

References

[1] S. Cacace and F. Camilli, *Ergodic problems for Hamilton-Jacobi equations: yet another but efficient numerical method*, preprint http://arxiv.org/abs/1601.07107.

[2] S. Cacace, F. Camilli and C. Marchi, *A numerical method for Mean Field Games on networks*, preprint http://arxiv.org/abs/1507.03731, accepted in ESAIM: M2AN.

[3] J.-M. Lasry and P.-L. Lions, *Mean field games*, Japanese Journal of Mathematics, 2 (1), 229–260, 2007.

An Hybrid control approach for the sailing route planning problem

Adriano Festa
RICAM - Austrian Academy of Sciences (ÖAW)
AltenbergerStrasse 4040 Linz, Austria
adriano.festa@oeaw.ac.at

Roberto Ferretti
Roma Tre - Universitá degli studi, Dipartimento di Matematica e Fisica - L.go S. Leonardo Murialdo, 1 00146 Roma, ferretti@mat.uniroma3.it

In the last half a century, the use of new technologies changed consistently the sport of sailing. This activity, became mainly not relevant from its commercial and military uses since the beginning of the XIX century, preserved a large interest from the purely sportive and technological development.
In this talk we deal with the aspect related to the route planning and the race strategy. A relevant contribution in it can be made using optimal control and differential games techniques.
To fix the ideas let us make a practical example of route planning. Following an objective of reaching a waypoint placed upwind (a buoy, for example) a sailing boat can not point directly the target. Simplifying a bit this is due to the fact that its speed is depending to the relative angle between the course and the direction of the wind (True Wind Angle TWA). Generally such speed is related to the TWA following a function (normally called polar plot, typically not convex). If we compute the optimal trajectory to reach the target using standard optimization techniques we obtain some unsatisfactory results coming from the non convexity of the dynamics. For this reason we propose to use a hybrid control approach [1] as presented for other purposes in [2]. We illustrate the advantages and the possible developments of the technique.

References

[1] S. Dharmatti and M. Ramaswamy. *Hybrid control systems and viscosity solutions*, SIAM journal on control and optimization 44.4 (2005) 1259–1288.

[2] R. Ferretti and H. Zidani. *Monotone numerical schemes and feedback construction for hybrid control systems*, Journal of Optimization Theory and Applications 165.2 (2015): 507–531.

Justification of macroscopic traffic flow model by specified homogenization of microscopic models

Nicolas Forcadel
Normandie Univ, INSA de Rouen, LMI 76000 Rouen
685 Avenue de l'Université, 76801 St Etienne du Rouvray cedex, France
nicolas.forcadel@insa-rouen.fr

Elisabetta Carlini
Sapienza Università di Roma
p.le Aldo Moro, 5, 00185 Roma, Italy
carlini@mat.uniroma1.it

Wilfredo Salazar
Normandie Univ, INSA de Rouen, LMI 76000 Rouen
685 Avenue de l'Université, 76801 St Etienne du Rouvray cedex, France
wilfredo.salazar@insa-rouen.fr

Mamdouh Zaydan
Normandie Univ, INSA de Rouen, LMI 76000 Rouen
685 Avenue de l'Université, 76801 St Etienne du Rouvray cedex, France
mamdouh.zaydan@insa-rouen.fr

The first goal of this talk is to present and to justify Hamilton-Jacobi formulation for macroscopic traffic flow model. The idea is to show how it is possible to deduce macroscopic models of traffic flow from microscopic ones. The main advantage of microscopic models (in which we describe the dynamics of each vehicle in an individual way) is that one can easily distinguish each vehicle and then associate different attributes (like maximal velocity, maximal acceleration...) to each vehicle. It is also possible to describe microscopic phenomena like red lights, slowdown or change of the maximal velocity. The main drawback is for numerical simulations where we have to treat a large number of data, which can be very expensive for example if we want to simulate the traffic at the scale of a town.
On the contrary, macroscopic models consist in describing the collective behavior of the vehicles for example by giving an evolution law on the density of vehicles. The oldest macroscopic model is the LWR model ([6, 7]), which dates back to 1955 and is inspired by the laws of fluid dynamics. More recently, some macroscopic models proposed to describe the flow of vehicles in terms of the averaged spacing between the vehicles (in some sense, the inverse of the density, see the work [5]). The main advantage of these macroscopic models is that it is possible to make numerical simulations on large portion of road. On the other side, it is more complicated to describe microscopic phenomena.
Generally speaking, microscopic models are considered more justifiable because the behavior of every vehicle can be described with high precision and it is immediately clear which kind of interactions are considered. On the contrary, macroscopic models are based on assumptions that are hardly verifiable. As a consequence, it is often desirable

establishing a connection between microscopic and macroscopic models so to justify the latter on the basis of the verifiable modeling assumptions of the former.
In the first part of this talk we will show how to pass from microscopic models to macroscopic ones. As we will explain, this problem can be seen as an homogenization result on a non-local Hamilton-Jacobi equation. More precisely, at the microscopic scale, we will consider a first order model of the type "follow the leader", i.e., the velocity of a vehicle depends only on the distance with the one in front of it and we will consider a local perturbation located at the origin which make slow down the vehicles. At the macroscopic scale, we attend to recover an Hamilton-Jacobi equation on the right and on the left of the origin and a condition of junction at the origin (as studied in [4]). This junction condition allows us to see the influence of the microscopic perturbation at the macroscopic scale.
In the second part of this talk we will present numerical scheme to solve this kind of Hamilton-Jacobi equations posed on networks. Recently, Costeseque, Lebacque and Monneau [1] propose a convergent finite difference scheme for HJ equations on networks and Imbert and Koumaiha [3] prove some error estimate for this scheme. In this talk, we will show how it is possible to use a semi-lagrangian algorithm for this problem. The difficulty here is to take into account the junction condition and in particular the fact that the hamiltonian can be different on different branches of the network.

Keywords specified homogenization, Hamilton-Jacobi equations, traffic flow, microscopic models, macroscopic models.

Acknowledgments Co-financed by the European Union with ERDF and by the Normandie Region.

References

[1] G. Costeseque, J.-P. Lebacque and R. Monneau, *A* convergent scheme for Hamilton-Jacobi equations on a junction: application to traffic, Numer. Math. 129 (3) (2015), 405-447.

[2] N. Forcadel, W. Salazar, *A* junction condition by specified homogenization of a discrete model with a local perturbation and application to traffic flow. Preprint

[3] C. Imbert and M. Koumaiha, *E*rror estimates for finite difference schemes associated with Hamilton-Jacobi equations on a junction. Preprint

[4] C. Imbert and R. Monneau, *L*evel-set convex Hamilton-Jacobi equations on networks. Preprint

[5] L. Leclercq, J.A. Laval and E. Chevallier, *T*he Lagrangian coordinates and what it means for first order traffic flow models. In ISTTT17, 2007.

[6] M. J. Lighthill and G. B. Whitham, *O*n kinematic waves. i. flood movement in long rivers, Proc. Roy. Soc. London. Ser. A, 229 (1955), p. 281-316.

[7] P. I. Richards, *S*hock waves on the highway, Operations Res., 4 (1956), p. 42-51.

A class of filtered scheme for second order Hamilton-Jacobi-Bellman equations

Athena Picarelli
University of Oxford
Andrew Wiles Building, Woodstock road, OX26GG, Oxford (UK)
athena.picarelli@maths.ox.ac.uk

Olivier Bokanowski
Laboratoire Jacques-Louis Lions, Université Paris-Diderot (Paris 7)
5 rue Thomas Mann, 75205 Paris Cedex 13
boka@math.jussieu.fr

Christoph Reisinger
University of Oxford
Andrew Wiles Building, Woodstock road, OX26GG, Oxford (UK)
christoph.reisinger@maths.ox.ac.uk

In this work we present a new class of high-order numerical schemes for second order time-dependent Hamilton-Jacobi-Bellman (HJB) equations. The equations considered involve possibly degenerated diffusions. Different ingredients are used. First, the idea introduced by Oosterlee in [5] and revisited, more recently, in [2] of using second order Backward Difference Formula (BDF2) approximation for the time discretization together with implicit schemes, showing good stability properties without CFL like conditions. Second, the policy iteration procedure to solve the related implicit discretized equations. However these first two steps lead to a non-monotone scheme, which prevents the use of the theoretical convergence results such as in [1]. Therefore on top of this we also use a "filtering" with a (low-order) monotone scheme to ensure convergence of the scheme, following the works [3] and [4]. With this suitable local modification we obtain a convergent scheme which is numerically of second order in time and space in the regular regions of the data. Numerical illustrations are presented on equations related to stochastic optimal control problems in mathematical finance.

References

[1] Barles, G. and Souganidis, P.E., 1991, *Convergence of approximation schemes for fully nonlinear second order equations*, Asymptotic Analysis, vol. 4, 271–283

[2] , Bokanowski, O. and Debrabant, K., 2016, *On multigrid for linear complementarity problems with application to American-style options*, Preprint

[3] Bokanowski, O. and Falcone, M. and Sahu, S. ,2015, *An efficient filtered scheme for some first order Hamilton-Jacobi-Bellman equations*, SIAM J. Scientific Computing, vol.38 (1), A171-A195

[4] Oberman, A. M. and Forese B. D., 2013, *Convergent filtered schemes for the Monge-Ampère partial differential equation*, SIAM J. Numerical Analysis , vol. 51, 423–444.

[5] Oosterlee, C. W., 2003, *On multigrid for linear complementarity problems with application to American-style options*, Electronic Transactions on Numerical Analysis, vol. 15, 165–185 (electronic)

Parabolic optimal control approaches for pedestrian dynamics

Marie-Therese Wolfram
University of Warwick
CV47AL Coventry, United Kingdom
m.wolfram@warwick.ac.uk

Martin Burger
WWU Münster
Einsteinstrasse 62, 48149 Münster, Germany
m.burger@wwu.de

Marco Di Francesco
University of L'Aquila Via Vetoio 1, 67100 L'Aquila, Italy
marco.difrancesco@univaq.it

Peter Markowich
Kaust and University of Vienna
Oskar-Morgenstern-Platz 1, 1090 Vienna, Austria
p.a.markowich@damtp.cam.ac.uk

In this talk we present an optimal control approach modelling fast exit scenarios in pedestrian crowds. In particular we consider the case of a large human crowd trying to exit a room as fast as possible. The motion of every pedestrian is determined by minimising a cost functional, which depends on his/her position, velocity, exit time and the overall density of people. This microscopic setup leads in the mean-field limit to a parabolic optimal control problem.
We discuss the modelling of the macroscopic optimal control approach and show how the optimal conditions relate to Hughes model for pedestrian flow. Furthermore we provide results on the existence and uniqueness of minimisers and illustrate the behaviour of the model with various numerical results.

Value function and optimal trajectories for a control problem with supremum cost function and state constraints

Hasnaa Zidani
ENSTA ParisTech, 828 Bd des Maréchaux, Palaiseau (France)
Hasnaa.Zidani@ensta-parsietch.fr

We study an aircraft abort landing problem formulated as a trajectory optimization problem with five dimensional state system, in presence of state constraints, and involving a maximum running cost function.
We are interested in studying a numerical approach based on Hamilton-Jacobi-Bellman theory. To do this, we develop new tools in the framework of HJB equations to handle in a rigorous way the state constraints.
Our approach is based on a reformulation of the problem in an auxiliary control problem free of state constraints (exact penalization). This step allow us to get a characterization of the epigraph of the value function without assuming any controllability assumption. Another tool that we develop in this study concerns some theoretical results for the trajectory reconstruction. In this topic, we introduce several procedures and prove their convergence. Several numerical experiments on the abort landing problem show the relevance of the theoretical results.

Heterogeneous domain decomposition methods: new results and perspectives

PROPOSERS

Gabriele Ciaramella
Université de Genève
Section de Mathématiques 2-4 rue du Lièvre, CH-1211 Genève
Gabriele.Ciaramella@unige.ch

Martin J. Gander
Université de Genève
Section de Mathématiques 2-4 rue du Lièvre, CH-1211 Genève
Martin.Gander@unige.ch

SPEAKERS

Mikel Landajuela
Université Paris 6 and Inria (Paris)
mikel.landajuela_larma@inria.fr

Paola Gervasio
Università degli Studi di Brescia
paola.gervasio@unibs.it

Martin J. Gander
Université de Genève
Martin.Gander@unige.ch

Franz Chouly
Université de Franche-Comté
franz.chouly@univ-fcomte.fr

Marc Alexander Schweitzer
Universität Bonn & Fraunhofer
schweitzer@ins.uni-bonn.de

Gabriele Ciaramella
Université de Genève
Gabriele.Ciaramella@unige.ch

In everyday scientific applications, scientists encounter problems that are heterogeneous "in nature" [4]. Typical examples of such problems are mechanical interaction of incompressible fluids with flexible structures, propagation of acoustic waves in heterogeneous media, aerodynamics applications, fluid dynamics and crystal growth processes; see, e.g., [4] for a review and [1, 2, 3] for recent mathematical developments.

Problems having a "heterogeneous nature" are very challanging from the mathematical and numerical analysis point of view, where a crucial issue is to develop techniques and

methods to obtain adequate matching conditions at the interface that separates the heterogeneous subregions.

In this minisymposium, recent advances of heterogeneous domain decomposition methods are discussed and new perspectives are posed in light of the most recent developments.

References

[1] Alauzet, Fabrèges, Fernández, Landajuela, *Nitsche-XFEM for the coupling of an incompressible fluid with immersed thin-walled structures* Computer Methods in Applied Mechanics and Engineering, Elsevier, 2016.

[2] Gander, Halpern, Martin, *A new Algorithm Based on Factorization for Heterogeneous Domain Decomposition*, to appear in Numerical Algorithms, 2016.

[3] Gander, Michaud, *Fuzzy Domain Decomposition: a new perspective on heterogeneous DD methods*, Domain Decomposition Methods in Science and Engineering XXI, Springer-Verlag, 2014.

[4] Quarteroni, Pasqarelli, Valli, *Heterogeneous Domain Decomposition: Principles, Algorithms, Applications*, Fifth International Symposium on Domain Decomposition Methods for PDEs, SIAM, 1991.

Nitsche-XFEM formulations and splitting schemes for the coupling of an incompressible fluid with immersed thin-walled structures

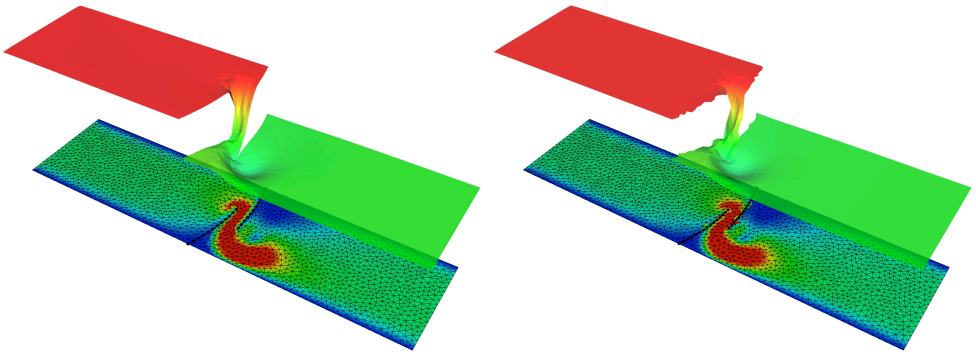
Mikel Landajuela
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
mikel.landajuela@polimi.it

Frédéric Alauzet
Inria Saclay
Rue Honoré d'Estienne d'Orves, 1 91120 - Palaiseau France
frederic.alauzet@inria.fr

Benoit Fabrèges
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
benoit.fabreges@polimi.it

Miguel A. Fernández
Inria Paris
Rue Simone Iff, 2 75012 - Paris France
miguel.fernandez@inria.fr

In this work we consider the mechanical interaction of an incompressible fluid with immersed thin-walled elastic structures. This is a widespread multi-physics problem that appears in a number of scientific and engineering fields: from the aeroelasticity of sailing boats and parachutes to the biomechanics of animal cells and physiological flows.
In order to address situations involving large structural deflections, with solids that might come into contact or that might break up, we combine an Eulerian formalism in the fluid with an unfitted mesh discretization, in which the solid mesh deforms independently of a background fixed fluid mesh. The thin-walled nature of the immersed solid introduces jumps on the fluid stresses which, respectively, results in weak and strong discontinuities of the velocity and pressure fields across the interface. The approximation spaces allow to capture these discontinuous features through suitable enrichment of the intersected elements (see [1]). The kinematic/dynamic fluid-solid interface conditions are enforced consistently using variants of Nitsche's method involving cut elements. Robustness with respect to arbitrary interface/element intersections is guaranteed through a ghost penalty stabilization (see [2]). For the temporal discretization, several splitting schemes with different degrees of fluid-solid decoupling (implicit, semi-implicit and explicit) are investigated. In particular, we address the extension of the explicit coupling paradigm introduced in [3] to the unfitted mesh framework. The stability and convergence properties of the methods proposed are rigorously analyzed in a representative linear setting. Several numerical examples, involving static and moving interfaces, illustrate the performance of the methods (see, e.g., Figure 1).



(a) ALE fitted (b) Nitsche-XFEM unfitted

Figure 1: Snapshots of the velocity field magnitude and pressure elevation obtained with an ALE based method (fitted meshes) and the present Nitsche-XFEM method (unfitted meshes).

References

[1] A. Hansbo and P. Hansbo. A finite element method for the simulation of strong and weak discontinuities in solid mechanics. Comput. Methods Appl. Mech. Engrg., 193(33-35):3523–3540, 2004.

[2] E. Burman and P. Hansbo, Fictitious domain methods using cut elements: III. A stabilized Nitsche method for Stokes problem. M2AN Math. Model. Numer. Anal., 48(3):859–874, 2014.

[3] M. Fernández, J. Mullaert, M. Vidrascu, Explicit Robin-Neumann schemes for the coupling of incompressible fluids with thin-walled structures, Comput. Methods Appl. Mech. Engrg. 267 (2013) 566–593.

An overlapping approach to couple Navier-Stokes and Darcy equations

Paola Gervasio
Università degli Studi di Brescia. via Branze, 38 25123 - Brescia Italy
paola.gervasio@unibs.it

Marco Discacciati
Loughborough University, Loughborough, LE11 3TU - United Kingdom
m.discacciati@lboro.ac.uk

Alessandro Giacomini
Università degli Studi di Brescia, via Branze, 38 25123 - Brescia Italy
alessandro.giacomini@unibs.it

Alfio Quarteroni
Ecole Polytechinque Fédérale de Lausanne, Station 8, CH-1015 - Lausanne Switzerland
alfio.quarteroni@epfl.ch

In this talk we consider the Navier-Stokes/Darcy problem modeling the filtration of incompressible fluids through porous media. To realize this coupling we use the so-called Interface Control Domain Decomposition (ICDD) method proposed in [1, 2]. The global computational domain is split into two overlapping subdomains in which we solve Navier-Stokes and Darcy equations, respectively, and the overlap corresponds to the transition region between the two regimes. ICDD introduces new auxiliary control variables on the subdomain internal boundaries (named interfaces) that play the role of the unknown traces of the Stokes velocity and Darcy pressure. Such controls are determined by minimizing a suitable cost functional that measures the jump of the quantities of interest at the interfaces of the decomposition. As a matter of fact we solve an optimal control problem in which both controls and observation are defined on the interfaces and whose constraints are the PDE's on the overlapping subdomains ([3]). In this talk we discuss both theoretical and computational aspects of the ICDD method applied to Stokes-Darcy coupling, and we show some numerical results with the aim of comparing our approach with classic coupling techniques based on non-overlapping decompositions and the Beavers-Joseph-Saffman interface conditions.

References

[1] M. Discacciati, P. Gervasio, and A. Quarteroni 2013 The interface control domain decomposition (ICDD) method for elliptic problems. SIAM J. Control Optim., vol. 51 (5), pp 3434-3458.

[2] M. Discacciati, P. Gervasio, and A. Quarteroni 2014 Interface control domain decomposition methods for heterogeneous problems. Int. J. Numer. Meth. Fluids. Vol. 76 (8), pp 471-496.

[3] M. Discacciati, P. Gervasio, A. Giacomini, and A. Quarteroni 2016 The interface control domain decomposition method for Stokes-Darcy coupling. SIAM J. Numer. Anal. vol. 54 (2), pp 1039-1068.

An Introduction to Heterogeneous Domain Decomposition, and a New Approach based on Factorization

Martin J. Gander
Université de Genève
Section de Matématique, Rue du Livre 2-4, CP 64, 1211 Genève 4, Switzerland
martin.gander@unige.ch

Heterogeneous domain decomposition methods, a terminology that was introduced in [22], are domain decomposition methods to solve problems which are using different models in different parts of the domain. There are two reasons for using different models for different regions: the first one is that there are problems where the physics is really different in different regions, and hence different models need to be used, for example in fluid-structure interaction, see [21, 5] and references therein. A very important area of application in this case is also the simulation of the cardiovascular system [10, 12], with the interaction between the blood and the arterial wall.
A second main area of heterogeneous domain decomposition methods is when homogeneous objects are simulated, but the partial differential equation modeling the physical phenomenon is too expensive to solve over the entire domain, and a simpler, less expensive model would suffice in most of the domain to reach the desired accuracy; air flow around an airplane is a typical example, where viscous effects are important close to the airplane, but can be neglected further away, see the early publication [6], and also [23, 4] and the references therein. An automatic approach for neglecting the diffusion in parts of the domain is the χ-formulation [2], and there are also techniques based on virtual control originating in [6], see [1] for the case with overlap, and [19] for the case without, and also [7, 8] for virtual control with variational coupling conditions. Transmission conditions for this situation have been developed in the seminal paper [17], but with the first situation described above in mind, i.e. there is indeed a viscous and an inviscid physical domain, and the coupling conditions are obtained by a limiting process as the viscosity goes to zero, see also [18], and [3] for an innovative correction layer. An important situation that fits also into this second area is the coupling of equations across dimensions, for example the blood flow in the artery can be modeled by a one dimensional model, but in the heart, it needs to be three dimensional, see for example [11].

After a brief introduction to heterogeneous domain decomposition methods, I will focus on the second case, i.e. where the global physical problem is indeed the same across the entire domain, but we want to use a heterogeneous domain decomposition method to be able to use a cheaper model in parts of the domain where the full model is not needed. Using as a model problem the coupling of an advection diffusion reaction equation to a pure advection reaction equation, I will first define a rigorous mathematical criterion which permits to measure the quality of a heterogeneous domain decomposition method [15]. I will then give a comparison of several heterogeneous domain decomposition methods from the literature, and also introduce a new approach based on operator factorization [20], whose underlying idea goes back the the PhD thesis of Dubach [9], see also [14]. The

results I will show for the steady case have appeared in [13], and for the unsteady case, see [16].

References

[1] V. Agoshkov, P. Gervasio, and A. Quarteroni. Optimal control in heterogeneous domain decomposition methods for advection-diffusion equations. *Mediterr. J. Math.*, 3(2):147–176, 2006.

[2] F. Brezzi, C. Canuto, and A. Russo. A self-adaptive formulation for the Euler-Navier Stokes coupling. *Comput. Methods Appl. Mech. Eng.*, 73:317–330, 1989.

[3] C. A. Coclici, W. L. Wendland, J. Heiermann, and M. Auweter-Kurtz. A heterogeneous domain decomposition for initial-boundary value problems with conservation laws and electromagnetic fields. In Tony Chan, Takashi Kako, Hideo Kawarada, and Olivier Pironneau, editors, *Twelfth International Conference on Domain Decomposition Methods, Chiba, Japan*, pages 281–288, Bergen, 2001. Domain Decomposition Press.

[4] Cristian A. Coclici and Wolfgang L. Wendland. Analysis of a heterogeneous domain decomposition for compressible viscous flow. *Mathematical Models and Methods in Applied Sciences*, 11(04):565–599, 2001.

[5] Simone Deparis, Marco Discacciati, Gilles Fourestey, and Alfio Quarteroni. Heterogeneous domain decomposition methods for fluid-structure interaction problems. In *Domain Decomposition Methods in Science and Engineering XVI*, pages 41–52. Springer, 2007.

[6] Q. V. Dinh, R. Glowinski, J. Périaux, and G. Terrasson. On the coupling of viscous and inviscid models for incompressible fluid flows via domain decomposition. In *First International Symposium on Domain Decomposition Methods for Partial Differential Equations (Paris, 1987)*, pages 350–369. SIAM, Philadelphia, PA, 1988.

[7] Marco Discacciati, Paola Gervasio, and Alfio Quarteroni. Heterogeneous mathematical models in fluid dynamics and associated solution algorithms. In *Multiscale and Adaptivity: Modeling, Numerics and Applications*, pages 57–123. Springer, 2011.

[8] Marco Discacciati, Paola Gervasio, and Alfio Quarteroni. The interface control domain decomposition (ICDD) method for elliptic problems. *SIAM Journal on Control and Optimization*, 51(5):3434–3458, 2013.

[9] Eric Dubach. *Contribution à la Résolution des Équations fluides en domaine non borné*. PhD thesis, Université Paris 13, 1993.

[10] L. Fatone, P. Gervasio, and A. Quarteroni. Numerical solution of vascular flows by heterogeneous domain decomposition methods. In Tony Chan, Takashi Kako, Hideo Kawarada, and Olivier Pironneau, editors, *Twelfth International Conference on Domain Decomposition Methods, Chiba, Japan*, pages 298–303, Bergen, 2001. Domain Decomposition Press.

[11] Luca Formaggia, Jean-Frédéric Gerbeau, Fabio Nobile, and Alfio Quarteroni. On the coupling of 3d and 1d Navier–Stokes equations for flow problems in compliant vessels. *Computer Methods in Applied Mechanics and Engineering*, 191(6):561–582, 2001.

[12] Luca Formaggia, Alfio Quarteroni, and Alessandro Veneziani. *Cardiovascular Mathematics: Modeling and simulation of the circulatory system*, volume 1. Springer, 2009.

[13] M. J. Gander, L. Halpern, C. Japhet, and V. Martin. Viscous problems with inviscid approximations in subregions: a new approach based on operator factorization. In *CANUM 2008*, volume 27 of *ESAIM Proc.*, pages 272–288. EDP Sci., Les Ulis, 2009.

[14] Martin J. Gander, Laurence Halpern, and Caroline Japhet. Optimized Schwarz algorithms for coupling convection and convection-diffusion problems. In *Proceedings of the 13th international conference of Domain Decomposition*, pages 253–260, 2001.

[15] Martin J. Gander, Laurence Halpern, Caroline Japhet, and Veronique Martin. Advection diffusion problems with pure advection approximation in subregions. In Olof B. Widlund and David E. Keyes, editors, *Domain Decomposition Methods in Science and Engineering XVI*, volume XVI of *Lecture Notes in Computational Science and Engineering 55*, pages 239–246. Springer-Verlag, 2007.

[16] Martin J. Gander, Laurence Halpern, and Veronique Martin. A new algorithm based on factorization for heterogeneous domain decomposition. *Numerical Algorithms*, 2016. to appear.

[17] Fabio Gastaldi and Alfio Quarteroni. On the coupling of hyperbolic and parabolic systems: Analytical and numerical approach. *Applied Numerical Mathematics 6*, 6:3–31, 1989.

[18] Fabio Gastaldi, Alfio Quarteroni, and Giovanni Sacchi Landriani. On the coupling of two dimensional hyperbolic and elliptic equations : Analytical and numerical approach. In T. Chan et al eds., editor, *Third International Symposium on Domain Decomposition Methods for Partial Differential Equations*, pages 22–63, Philadelphia, 1990. SIAM.

[19] P. Gervasio, J.-L. Lions, and A. Quarteroni. Heterogeneous coupling by virtual control methods. *Numer. Math.*, 90(2):241–264, 2001.

[20] J.-P. Lohéac, F. Nataf, and M. Schatzman. Parabolic approximations of the convection-diffusion equation. *Math. Comp.*, 60(202):515–530, 1993.

[21] H. J.-P. Morand and R. Ohayon. *Fluid Structure Interaction*. John Wiley & Sons, 1995.

[22] A. Quarteroni, F. Pasquarelli, and A. Valli. Heterogeneous domain decomposition principles, algorithms, applications. In David E. Keyes, Tony F. Chan, Gérard A. Meurant, Jeffrey S. Scroggs, and Robert G. Voigt, editors, *Fifth International Symposium on Domain Decomposition Methods for Partial Differential Equations*, pages 129–150, Philadelphia, PA, 1992. SIAM.

[23] A. Quarteroni and L. Stolcis. Homogeneous and heterogeneous domain decomposition for compressible fluid flows at high Reynolds numbers. *Numerical Methods for Fluid Dynamics*, 5:113–128, 1995.

A Schwarz waveform relaxation method for parabolic-hyperbolic coupling in 1D

Franz Chouly
LMB - Université de Franche-Comté
16 route de Gray, 25000 Besançon, FRANCE
franz.chouly@univ-fcomte.fr

Pauline Klein
LMB - Université de Franche-Comté
16 route de Gray, 25000 Besançon, FRANCE
pauline.klein@univ-fcomte.fr

We present a Schwarz waveform relaxation method [3, 4] for the coupling between the heat equation and the wave equation in 1D, as a prototype of fluid-structure interaction problem [5]. We focus first on the idealized case of unbounded heat and wave domains, or, equivalently, bounded domains with artificial boundary conditions. Following the methodology described in, e.g., [2], we derive optimized conditions that improve the convergence of the coupling algorithm. Each sub-problem is then discretized with finite elements in space and standard time-marching schemes in time (backward Euler, Crank-Nicolson), as this is the case in most of the current numerical methods for fluid-structure interaction [1]. Some preliminary numerical results are discussed as well.

References

[1] Fernández, M.A. 2011. *Coupling schemes for incompressible fluid-structure interaction: implicit, semi-implicit and explicit*. SeMA Journal. 55(1), 59–108.

[2] Gander, M.J. 2006. *Optimized Schwarz methods*. SIAM J. Numer. Anal. 44(2), 699–731.

[3] Gander, M.J. and Stuart, A.M. 1998. *Space-time continuous analysis of waveform relaxation for the heat equation*. SIAM J. Sci. Comp. 19(6), 2014–2031.

[4] Giladi, E. and Keller, H.B. 2002. *Space-time domain decomposition for parabolic problems*. Numer. Math. 93(2), 279–313.

[5] Zhang, X. and Zuazua, E. 2007. *Long-time behavior of a coupled heat-wave system arising in fluid-structure interaction*. Arch. Ration. Mech. Anal. 184(1), 49–120.

Partition of Unity Methods

Marc Alexander Schweitzer
Rheinische Friedrich-Wilhelms-Universität Bonn & Fraunhofer SCAI
Wegelerstr. 6, D-53115 Bonn, Germany
schweitzer@ins.uni-bonn.de

Sa Wu
Rheinische Friedrich-Wilhelms-Universität Bonn
Wegelerstr. 6, D-53115 Bonn, Germany
wu@ins.uni-bonn.de

Albert Ziegenhagel
Fraunhofer SCAI
Schloss Birlinghoven, D-53754 Sankt Augustin, Germany
albert.ziegenhagel@scai.fraunhofer.de

In this talk, we focus on partition of unity (PU) based generalizations of the finite element method (GFEM) [4, 2] and discuss issues of stability and conditioning of the resulting stiffness matrix due to enrichment [3]. We present a general approach to automatically construct a stable basis for arbitrary enrichments and an appropriate multilevel solver when the employed partition of unity satisfies the flat-top property [1]. Moreover, we present a general construction for lumped mass matrices for enriched and higher order GFEM under the assumption that the employed PU is non-negative [5]. We present some numerical results from structural mechanics and fluid dynamics to show the effectiveness of the presented approach in application settings.

References

[1] M. Griebel and M. A. Schweitzer, *A Particle-Partition of Unity Method—Part III: A Multilevel Solver*, SIAM Journal on Scientific Computing **24** (2002), no. 2, 377–409.

[2] M. A. Schweitzer, *Meshfree and Generalized Finite Element Methods*, Habilitation, Institute for Numerical Simulation, University of Bonn, 2008.

[3] _____, *Stable Enrichment and Local Preconditioning in the Particle–Partition of Unity Method*, Numer. Math. **118** (2011), no. 1, 137–170.

[4] _____, *Generalizations of the finite element method*, Central European Journal of Mathematics **10** (2012), 3–24.

[5] _____, *Variational mass lumping in the partition of unity method*, SIAM Journal on Scientific Computing **35** (2013), no. 2, A1073–A1097.

A Partition of Unity Method for Heterogeneous Domain Decomposition Problems

Gabriele Ciaramella
Université de Genève
Section de Mathématiques 2-4 rue du Lièvre, CH-1211 Genève
Gabriele.Ciaramella@unige.ch

Martin J. Gander
Université de Genève
Section de Mathématiques 2-4 rue du Lièvre, CH-1211 Genève
Martin.Gander@unige.ch

In many applications, mathematical and numerical models involve simultaneously more than one single phenomenon; see, e.g., [3] and references therein. In this situation different equations are adapted in the overlapping subregion of the domain in order to approximate the physical model and obtain an efficient reduction of the computational cost. The coupling between the different equations must be carefully handled to guarantee accurate results.
In this talk, we present a new method that allows to design an efficient coupling between the different equations. This new heteorgenous domain decomposition mathod is based on the partition partition of unity framework, that has been introduced in the seminal work [1] and used as a powerful technique for the accurate solution of complicated PDEs problems; see, e.g., [2] and other related works. We show that our new method allows to couple equations of different types and has the special feature to be embedded in an optimization framework, which allows us to design efficient couplings between the considered differential equations. Numerical experiments demonstrate the efficieny of the proposed framework.

References

[1] Babuska, Melenk, *The partition of unity method*, Int. J. Num. Methods in Eng. 1997.

[2] Griebel, Schweitzer, *A particle-parition of unity method for the solution of elliptic, parabolic, and hyperbolic PDEs*, SIAM J. Sci. Comp. 2000.

[3] Quarteroni, Pasqarelli, Valli, *Heterogeneous Domain Decomposition: Principles, Algorithms, Applications*, Fifth International Symposium on Domain Decomposition Methods for PDEs, SIAM, 1991.

Numerical Methods for PDEs in Networks

PROPOSERS

Christian Contarino
Università degli Studi di Trento
via Sommarive, 14 38123 - Povo (Trento) Italy
christian.contarino@unitn.it

Eleuterio F. Toro
Università degli Studi di Trento
Via Mesiano, 77 38123 - Mesiano (Trento) Italy
eleuterio.toro@unitn.it

SPEAKERS

Raul Borsche (keynote)
Technische Universität Kaiserslautern
borsche@mathematik.uni-kl.de

Jochen Kall
Technische Universität Kaiserslautern
kall@mathematik.uni-kl.de

Christian Contarino
Dipartimento di Matematica, Università degli Studi di Trento
christian.contarino@unitn.it

M. Elena Vázquez Cendón
Departamento de Matemática Aplicada, Santiago de Compostela
elena.vazquez.cendon@usc.es

Sébastien Boyaval
Laboratoire d'hydraulique Saint-Venant, Paris
sebastien-externe.boyaval@edf.fr

In recent years, the construction of suitable numerical methods for solving Partial Differential Equations (PDEs) in domains consisting of networks of one-dimensional sub-domains has become the subject of much research activity. Related practical applications include gas flow in pipes, traffic flow, water flow in networks of channels and blood flow in the human circulation. In all of these applications, a crucial point is the coupling of the information coming from different sub-domains and converging to a single point, here called a junction. Devising numerical methods for junctions is therefore essential to simulate realistic fluid networks. There exists a wide variety of numerical techniques to treat junctions. For instance, one can couple one-dimensional flow models with a local multidimensional model, preserving geometrical information, such as angles, as well as momentum and energy. One can also solve a Riemann problem at a junction and use the solution in a Godunov-type numerical scheme. It is also possible to locally use a compartmental model that accounts for more complex behaviour via a system of

Ordinary Differential Equations (ODEs). Although the literature is growing, there are still mathematical and numerical aspects to be addressed.

This minisymposium aims at gathering experts in theoretical aspects and in numerical methods for PDEs in networks, as well as applications.

Kinetic and related macroscopic models for chemotaxis on networks

Raul Borsche
University of Kaiserslautern
borsche@mathematik.uni-kl.de

Axel Klar
University of Kaiserslautern

T.N.H. Pham
University of Kaiserslautern

In this talk we will develop coupling conditions for the kinetic chemotaxis equations and derive from these equations coupling condition for the macroscopic Cattaneo and half-moment models. These coupling conditions guarantee on the one hand the conservation of mass through nodes, and on the other hand, they satisfy a positivity condition for the density. These hyperbolic equations, as in [1, 2], require an approach to the coupling conditions which is different to the Keller-Segel context. However, in the diffusive limit, when the scaling parameter goes to 0, all coupling conditions converge to those of the Keller-Segel model, i.e. the conservation of mass through nodes and a continuity condition. With the help of asymptotic preserving schemes [3] we investigate the kinetic equations, the Cattaneo equations and the half-moment models on a single line. Combining this with a numerical method to solve the coupling problem at junctions the dynamics of the different models on complex networks can be analysed in several test cases.

References

[1] G. Bretti, R. Natalini and M. Ribot, 2014 'A hyperbolic model of chemotaxis on a network: a numerical study', *M2AN*, 48 no. 1, pp. 231-258

[2] F.R. Guarguaglini and R. Natalini, 2015 'Global smooth solutions for a hyperbolic chemotaxis model on a network', *SIAM J. Math. Anal.*, 47 no. 6, pp. 4652-4671

[3] S. Jin, L. Pareschi and G. Toscani, 1998 'Diffusive relaxation schemes for multiscale discrete-velocity kinetic equations', *SIAM J. Numer. Anal.*, 35 no. 6, pp. 2405–2439

ADER Schemes for Systems of PDEs on Networks coupled with ODEs

Jochen Kall
Technische Universität Kaiserslautern
Erwin-Schrödinger-Straße 48, 67663 Kaiserslautern, Germany
kall@mathematik.uni-kl.de

Raul Borsche
Technische Universität Kaiserslautern
Erwin-Schrödinger-Straße 48, 67663 Kaiserslautern, Germany
borsche@mathematik.uni-kl.de

Modeling the behavior of fluids or gases in networks, e.g. gas pipelines, district heating, water and wastewater networks, canals, blood flow, etc, leads to systems of conservation laws coupled at vertices, sometimes including ODEs. We present a generalization of the ADER scheme of Toro-Castro type to such networks with ODE coupling vertices, discuss advantages and disadvantages of the approach compared to HEOC type solvers, and test the method at several numerical examples.

Junction-Generalized Riemann Problem for Stiff Hyperbolic Balance Laws in Networks of Blood Vessels

Christian Contarino
Università degli Studi di Trento
via Sommarive, 14 38123 - Povo (Trento) Italy
christian.contarino@unitn.it

Eleuterio F. Toro
Università degli Studi di Trento
eleuterio.toro@unitn.it

Gino I. Montecinos
Universidad de Chile
gmontecinos@dim.uchile.cl

Raul Borsche
Technische Universität Kaiserslautern
borsche@mathematik.uni-kl.de

Jochen Kall
Technische Universität Kaiserslautern
kall@mathematik.uni-kl.de

We design a new implicit solver for the Junction-Generalized Riemann Problem (J-GRP) [3], which is based on a recently proposed implicit method for solving the Generalized Riemann Problem (GRP) for systems of hyperbolic balance laws [5]. We use the new J-GRP solver to construct an ADER scheme that is globally explicit, locally implicit and with no theoretical accuracy barrier, in both space and time. The resulting ADER scheme is able to deal with stiff source terms and can be applied to non-linear systems of hyperbolic balance laws in domains consisting on networks of one-dimensional sub-domains. Here we specifically apply the numerical techniques to networks of blood vessels. An application to a physical test problem consisting of a network of 37 compliant silicon tubes (arteries) and 21 junctions, reveals that it is imperative to use high-order methods at junctions, in order to preserve the desired high-order of accuracy in the full computational domain. For other similar numerical techniques, see [2, 4, 1]

References

[1] Banda, M. K., Häck, A. S., and Herty, M. (2015). *Numerical Discretization of Coupling Conditions by High-Order Schemes.*

[2] Borsche, R., and Kall, J. (2014). *ADER schemes and high order coupling on networks of hyperbolic conservation laws.* Journal of Computational Physics, 273, 658-670.

[3] Contarino, C., Toro, E. F., Montecinos, G. I., Borsche, R., and Kall, J. (2016). *Junction-Generalized Riemann Problem for stiff hyperbolic balance laws in networks: An implicit solver and ADER schemes.* Journal of Computational Physics, 315, 409-433.

[4] Müller, L. O., and Blanco, P. J. (2015). *A high order approximation of hyperbolic conservation laws in networks: Application to one-dimensional blood flow.* Journal of Computational Physics, 300, 423-437.

[5] Toro, E. F., and Montecinos, G. I. (2015). *Implicit, semi-analytical solution of the generalized Riemann problem for stiff hyperbolic balance laws.* Journal of Computational Physics, 303, 146-172.

Finite volume solution of gas flow in networks: numerical treatment of junctions

M. Elena Vázquez-Cendón
Universidade de Santiago de Compostela, ITMATI
Departamento de Matemática Aplicada, Universidade de Santiago de Compostela, 15706 Santiago de Compostela, Spain
elena.vazquez.cendon@usc.es

Alfredo Bermúdez
Universidade de Santiago de Compostela, ITMATI
Departamento de Matemática Aplicada, Universidade de Santiago de Compostela, 15706 Santiago de Compostela, Spain
alfredo.bermudez@usc.es

Xián López
Universidade de Santiago de Compostela, ITMATI
Departamento de Matemática Aplicada, Universidade de Santiago de Compostela, 15706 Santiago de Compostela, Spain
xian.lopez@usc.es

Managing gas transport networks is a Mathematical modelling is an important subject in planning and operating gas transportation networks which is complex problem because of the great number of possibilities to routing the gas through the pipes (see reference books, [8], [11]).

Most papers and computer programs on the subject deal with the case of steady state. Based on steady state models, network optimization problems have been considered that, in particular, aim at saving operation costs related to the self consumption of gas in compression stations, needed to compensate the pressure loss due to pipe wall friction (see [1], [11]). However, less papers have been devoted to transient models (see, for instance, [4], [5], [2], for one single pipe, or [9], [10] and [6] for networks).

The present work deals with the numerical solution by finite volume methods of transient mathematical models of gas transport networks. The model consists of a system of nonlinear hyperbolic partial differential equations coupled at the nodes of the network whose topology is modelled by a direct graph. The edges of the graph represent pipes where the gas flow is modelled by the non-isothermal non-adiabatic Euler compressible equations for real gases, with source terms arising from heat transfer with the outside of the network, wall viscous friction, and gravity force; the latter involving the slope of the pipe.

In a previous paper, [2], the authors consider one single pipe and introduce a finite volume scheme for the corresponding model. Upwind discretization of the flux is done by using the Q-scheme of van Leer. Moreover, in order to get a well-balanced scheme the source terms are discretized by making some upwinding similar to the one in the flux term, following the general methodology proposed in [3].

As a step further, the main goal of this presentation is to consider a network. This

requieres to deal with the junctions where the one-dimensional gas dynamic equations for pipes converging at the junction are coupled. The proposed technique consist in using one-dimensional models for the pipes with two-dimensional models for the junctions.

References

[1] A. Bermúdez, J. González-Díaz, F.J. González-Diéguez, A.M. González-Rueda, M.P. Fernández de Córdoba. 2015 *Simulation and optimization models of steady-state gas transmission networks*, Energy Procedia. 64,130–139.

[2] A. Bermúdez, X. López, M.E. Vázquez-Cendón. 2016 *Numerical solution of non-isothermal non-adiabatic flow of real gases in pipelines*. Sumitted to Journal of Computational Physics.

[3] A. Bermúdez, M.E. Vázquez-Cendón. 1994 *Upwind methods for hyperbolic conservation laws with source terms*. Computers and Fluids. 23, 1049–1071.

[4] J. Brouwer, I. Gasser, M. Herty. 2011 *Gas pipeline models revisited: model hierarchies, nonisothermal models, and simulations of networks*. Multiscale Model. Simul. 9, no. 2, 601–623.

[5] S. Elaoud, E. Hadj-Taiëb. 2008 *Transient flow in pipelines of high-pressure hydrogen–natural gas mixtures*. Int. J. of Hydrogen Energy. 33, 4824–4832.

[6] B. Geissler, O. Kolb, J. Lang, G. Leugering, A. Martin and A. Morsi. 2001 *Mixed integer linear models for the optimization of dynamical transport networks*, Math Meth Oper Res 73, 339–362.

[7] R. Käppeli, S. Mishra. 2014 *Well-balanced schemes for the Euler equations with gravitation*. Journal of Computational Physics. 259, 199–219.

[8] T. Kosch, B. Hiller, M.E. Pfetsch, L. Schewe Eds. 2015 *Evaluating Gas Network Capacities*. SIAM, Philadelphia.

[9] M. Herty. 2007 *Modelling, simulation and optimization of gas networks with compressors*. Networks and Heterogeneous Media. 2, 81–97.

[10] A. Morin, G. A. Reigstadb. 2015 Pipe networks: coupling constants in a junction for the isentropic Euler equations. Energy Procedia 64, 140–149.

[11] A.J. Osiadacz. 1987 *Simulation and Analysis of Gas Networks.* Gulf Publishing Company, Houston.

River modelling with a network of 1D open channels

Sébastien Boyaval
Laboratoire d'hydraulique Saint-Venant (Ecole des Ponts ParisTech – EDF R&D , CEREMA)
Université Paris-Est, Chatou France& MATHERIALS, INRIA
sebastien.boyaval@enpc.fr

Nicole Goutal
Laboratoire d'hydraulique Saint-Venant (EDF R&D – Ecole des Ponts ParisTech , CEREMA)
Université Paris-Est, Chatou France & ANGE, INRIA
nicole.goutal@edf.fr

The nonlinear Shallow Water Equations (SWE) proposed by A.B. de Saint-Venant as a one-dimensional-in-space free-surface flow model are widely used in hydraulic engineering for the prediction of water levels.
Given an open channel, the 1D SWE only describe the time evolutions of the cross-sectional area and of the water discharge, quite crudely (in comparison with e.g. the free-surface Navier-Stokes equations). But they can be solved very efficiently for e.g. flood forecasting and dam-break wave, when supplemented with initial and boundary conditions.
Now, rivers are often made of a main stream channel plus distributary and tributary channels. For the purpose of numerical simulation, a number of river systems have been modelled as networks of 1D open channels governed by SWE connected through junctions (confluences). Various equations have been added at the junctions by practitionners to set a well-posed evolution problem.
In this talk, we explain how junctions are handled in the software Mascaret[1] [1] which is currently used in France by EDF, CEREMA and SCHAPI among others to manage hydraulic structures or forecast floods on some French rivers (Garonne, Loire, Seine…). We also discuss some mathematical and physical issues raised by the chosen junction models.

From the physical viewpoint, the choice of a junction model that connects the cross-sectional areas and the water discharges in different intersecting branches can obviously not take into account all the processes occuring at small scale. The choice of a junction model therefore favours some macroscopic trend like the continuity of smooth variables (such as the water elevation when the flow remains subcritical) and first principles like mass conservation (implying an equation for the discharges). The problem is: how to devise a model that encompasses various flow regimes (including transcritical) and can be used numerically for operational purposes.

From the mathematical viewpoint, the (discrete) network model has to be well-posed in numerical practice, that is when supplemented with realistic initial and boundary conditions. Now, there is still not a well-established theory for generalized Riemann problems at a junction connecting 1D hyperbolic systems of conservation laws like SWE. However, a number of schemes are efficiently used in practice. Are they reliable?

[1] www.opentelemac.org

References

[1] Maurel, F. 1996 *Traitement des confluents dans le logiciel Mascaret* EDF internal report HE-43/96/067/A

Numerical Methods and Algorithms for Data Analysis in Science and Engineering Applications

PROPOSERS

Salvatore Cuomo
University of Naples Federico II
via Cintia, 80126 - Naples, Italy
salvatore.cuomo@unina.it

Ardelio Galletti
University of Naples "Parthenope"
Centro Direzionale, isola C4 8043 - Naples, Italy
ardelio.galletti@uniparthenope.it

Livia Marcellino
University of Naples "Parthenope"
Centro Direzionale, isola C4 8043 - Naples, Italy
livia.marcellino@uniparthenope.it

SPEAKERS

Emanuele Brugnoli
Dept. of Mathematics and Computer Science - University of Palermo
emanuele.brugnoli@unipa.it

Rosanna Campagna
Dept. Mathematics and Applications, University of Naples Federico II
rosanna.campagna@unina.it

Giovanna Califano
Dept. of Mathematics, University of Salerno
gcalifano@unisa.it

Antonio Cicone
Dept. of Information Engineering, Computer Science and Mathematics University of L'Aquila
antonio.cicone@univaq.it

Antonio Maratea
Dept. of Science and Technology, University of Naples "Parthenope"
antonio.maratea@uniparthenope.it

Martina Moccaldi
Dept. of Mathematics, University of Salerno
martina.moccaldi@unisa.it

The extraction and the assessment of useful information from the huge amount of data available in Bioinformatics, Neurosciences, Cloud Web Services or Climate modelling poses many challenges and difficulties. The goal of the minisymposium will be to approach and discuss recent trends in data mining, focusing on the analysis and the classification of large

data sets using novel methods, numerical models and efficient and reliable algorithmic strategies belonging to the family of clustering and genetic algorithms, neural networking and regression analysis. In particular, we are interested in the emerging techniques for data analysis addressed to relevant real-world applications, in order to share ideas, experiences and research results. The topics include, but are not limited to, problems related to Signal Processing, Multi-variate Analysis and Classification, Distributed Computing for e-Health, Machine Learning in Social Systems.

References

[1] J Han, M Kamber, J Pei - *Data mining: concepts and techniques.* Third Edition (The Morgan Kaufmann Series in Data Management Systems), 2011.

[2] Hair, J.F. - *Multivariate data analysis.* Pearson Prentice Hall, 2006.

Iterative Methods for Signal Reconstruction on Graphs

Emanuele Brugnoli
Dipartimento di Matematica e Informatica - Università degli Studi di Palermo
via Archirafi, 34 90123 - Palermo Italy
emanuele.brugnoli@unipa.it

Elena Toscano
Dipartimento di Matematica e Informatica - Università degli Studi di Palermo
via Archirafi, 34 90123 - Palermo Italy
elena.toscano@unipa.it

Calogero Vetro
Dipartimento di Matematica e Informatica - Università degli Studi di Palermo
via Archirafi, 34 90123 - Palermo Italy
calogero.vetro@unipa.it

In applications such as social, energy, transportation, sensor, and neuronal networks, big data naturally reside on the vertices of graphs. Each vertex stores a sample, and the collection of these samples is referred to as a graph signal. The product of the network graph with the time series graph is considered as underlying structure for the evolution through time of graph signal "snapshots". The framework of *signal processing on graphs* [4] extends concepts and methodologies from classical discrete signal processing. The task of sampling and recovery is one of the most critical topics in the signal processing community.
In this talk, we present some localized iterative methods, obtained by modifying the Marvasti algorithm [2] in classical signal processing, for interpolating graph signals from only a partial set of samples, both in vertex and time domain. Our methods are also compared with other recent algorithms [3, 5] in order to study rate of convergence and computational efficiency [1]. The experimental results demonstrate the effectiveness of the proposed reconstruction methods in real world datasets and noisy scenarios.

References

[1] Berinde, V. 2007 *Iterative approximation of fixed points*, 2nd ed., Springer.

[2] Marvasti, F.; Analoui, M. and Gamshadzahi, M. 1991 *Recovery of Signals from Nonuniform Samples Using Iterative Methods*. IEEE Trans. Sig. Proc. 39 (4), 872–878.

[3] Narang, S. K.; Gadde, A., Sanou, E. and Ortega, A. 2013 *Localized iterative methods for interpolation in graph structured data*. Proc. 1st IEEE Global Conf. Signal Inf. Process. (GlobalSIP), 491–494.

[4] Shuman, D. I.; Narang, S. K.; Frossard, P.; Ortega, A. and Vandergheynst, P. 2013 *The emerging field of signal processing on graphs: Extending high-dimensional data*

analysis to networks and other irregular domains. IEEE Trans. Sig. Proc. Mag. 30 (3), 83–98.

[5] Wang, X.; Liu, P. and Gu, Y. 2015 *Local-Set-Based Graph Signal Reconstruction*. IEEE Trans. Sig. Proc. 63 (9), 2432–2444.

Using RBF-FD to solve a differential problem of singular type flow in hydrology

Rosanna Campagna
University of Naples "Parthenope"
Department of Science and Technology, Centro Direzionale, Isola C4, 80143, Naples, Italy
rosanna.campagna@uniparthenope.it

Flows generated by single (distributed) sources such as flows generated by wells are of central interest in hydrology. Many solutions for such flows have been derived for different configurations in homogeneous [6] as well as layered aquifers (e.g., [7]). These solutions have served as a basis for solving many practical problems. Actually, natural porous formations are heterogeneous, with their transmissivity varying in the space quite irregularly [2]. In this paper, we are concerned with modeling of steady water flow at regional scale. By regional scale, we refer to entire aquifers (or major parts) that are characterized by horizontal scales much larger than the formation thickness. At this scale, it is customary to model the flow as two dimensional in the horizontal plane by averaging the head and specific discharge over the thickness.
At stationary conditions, an elliptic PDE is the mathematical model describing the hydraulic head with respect to the water surface in the well; in this model the well represents a *singular-type flow* so a Dirac delta function δ is assumed to describe the effects of the extraction on the piezometric height. The solution is request to be a continuous function.
A new numerical approach is presented in which a scheme *Finite Difference (FD)-like* is applied to a totally unstructured node distribution; this is possible by approximating the successive differential operators through a linear combination of functions belonging to a suitable *Radial basis*. Such an approach is particularly attractive taking into account the possible presence of "obstacles" or sites where a sampling is impossible or, even, forbidden, in the surrounding of the well (e.g. a river, a waste dump, a building,...).

We solve the problem consisting in the groundwater equation (in the hypothesis of extensive aquifer [8, 9]), with a suitable boundary condition. In polar coordinates it becomes:

$$\mathbf{M}(\mathbf{P}) : \begin{cases} \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial h}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 h}{\partial \theta^2} = -\frac{Q}{T}\frac{1}{2\pi r}\delta(r) & (r,\theta) \in \Omega \\ h(r,\theta) = h^B & (r,\theta) \in \partial\Omega \end{cases} \tag{1}$$

where Q is the rate of flow through an arbitrary cross-section (of the well), T represents the transmissivity of the aquifer for horizontal flow, γ is the specific weight of the water; we set $\gamma = 1$. It is a realistic assumption let h goes towards zero, when the distance from the well grows up. Some issues arise in the numerical solution of in this problem:

(a) the numerical modeling of the Dirac delta δ; this will affect the boundary condition around the well;

(b) the numerical scheme to approximate derivatives.

Joint research topics with: Prof. Giulio Giunta (University of Naples "Parthenope") and Prof. Gerardo Serverino (University of Naples Federico II)

The point (a) has been dealt with by following [10]. As concerned the point (b), a FD scheme has been used, since it is widly used in large-scale simulations in many applications areas, such as geophysical fluid dynamics. We focus on the idea to integrate FD approach with the new emerging *Radial Basis Function Finite Difference (RBF-FD)* scheme.
Firstly a discretization for the differential operators is introduced; a circular grid excluding the singular-type point is set; the fixed node locations are such $\mathbf{s}_{i,j} = (r_i, \theta_j)$, $i, j = 1, \ldots, n+1$; the five-point Laplacian scheme, furnishes a FD second order approximation for second order derivaties:

$$\mathbf{M_h}(\mathbf{P}) : \begin{cases} \frac{h_{i+1,j}-2h_{i,j}+h_{i-1,j}}{\Delta_r^2} + \frac{1}{i\Delta_r}\frac{h_{i+1,j}-h_{i-1,j}}{2\Delta_r} + \\ + \frac{1}{(i\Delta_r)^2}\frac{h_{i,j+1}-2h_{i,j}+h_{i,j-1}}{\Delta_\theta^2} = -\frac{Q}{T}\frac{1}{2\pi r_i}\tilde{\delta}_i, \\ i = 1, \ldots, m, \quad j = 0, \ldots, n+1, \\ h_{1,j} = -\frac{Q}{T}\frac{1}{2\pi}\frac{1}{\Delta_r^2} \\ h_{m+1,j} = 0 \end{cases} \tag{2}$$

where Δ_r is the radial step in the structured grid. The solution in heterogeneous soils requires a stochastic parametrization of the transmissivity field. The randomness of the hydraulic transmissivity induces the randomness of the hydraulic head. In Fig.1 there is an example of solution of (2) computed by a prototipal software module developed by the authors.
It's well known that in FD formulae the successive differential operators at a given point are approximated as linear combinations of its values at some equispaced nodes, where unknown weights are computed by polynomial interpolation. In these scheme the grid points are imposed to belong to a *structureted grid*. This constraint strongly limits the geometric flexibility of the method. A RBF-FD scheme allows to overcome this drawnback. RBF, originated as a technique for interpolation of multidimensional scattered data, became popular as a mesh-free method for the solution of PDEs on irregular domains [4, 5]. Being entirely mesh-free, RBF-FD discretizations are suitable when local refinements or scattered nodes are needed. For example, RBF-FD can successfully be used to deal with the heterogeneity and irregularity of the domain surrounding the well. This opportunity let's hope that the accuracy of the solution will improve. A brief survey on the evolution of RBFs and the application of RBF/RBF-FD discretizations for solving large-scale benchmark problems, mostly from geoscience, is in [3].
Let $\mathbf{x}_1, \ldots, \mathbf{x}_N$ be a stencil consisting of N *scattered nodes* and $\mathcal{L}$ a differential operator. For a given node, say $\mathbf{x}_1$, the objective is to approximate $\mathcal{L}u(\mathbf{x}_1)$ as a linear combination of the values of u at the N scattered nodes, so that

$$\mathcal{L}u(\mathbf{x}_1) \approx \sum_{i=1}^{N} \alpha_i u(\mathbf{x}_i) \tag{3}$$

The weighting coefficients α_i are computed by setting a suitable RBF, ϕ_i, $i = 1, \ldots, N$ and then by assuming the following approximation:

$$\mathcal{L}u(\mathbf{x}_1) \approx \mathcal{L}\phi_j(\mathbf{x}_1)$$

with

$$\mathcal{L}\phi_j(\mathbf{x}_1) = \sum_{i=1}^{N} \alpha_i \phi_j(\mathbf{x}_i), \quad j = 1, \ldots, N \tag{4}$$

The (4) is a system of N linear equations on N unknowns, solved by linear interpolation of the RBF in the scattered nodes. The computed weights can be used in the approximation

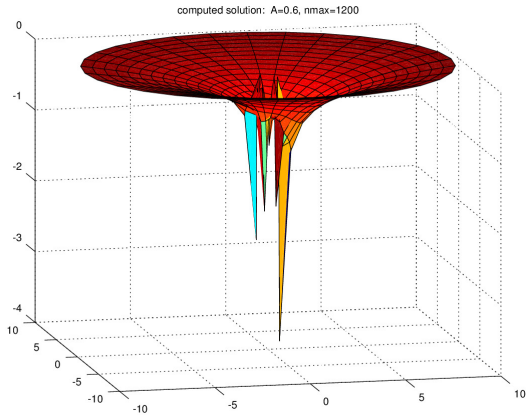


Figure 1: An example of computed solution.

(3) so furnishing the weighted FD formulas. How to derive the exact RBF-FD formulas for first and second derivatives is in [1]. RBF are generally characterized by the presence of a *shape parameter*. In [1], it is proved that an optimal value of the shape parameter for which the discretization error is minimum can be found. This allow to improve the accuracy granted by the FD schemes.
The choice of the Radial basis $\{\phi_j\}_{j=1,\dots,N}$ is critical. In our problem the solution is meaningful around the well while tends to zero far from it (see Fig.1); moreover it must be a continuous function in the whole domain; a possible choice can be the infinitely smooth RB Gaussian functions:

$$\phi(d = \|\mathbf{x} - \mathbf{x}_k\|) = e^{-(\varepsilon d)^2}$$

where ε is the shape parameter and the norm is the Euclidean distance function. Finally, we are working to define a new radial basis that better fits the specific data from the problem in exam.

References

[1] Bayona V., Moscoso M., Carretero M., Kindelan M. (2010), *RBF-FD formulas and convergence properties*, Journal of Computational Physics, Volume 229, Issue 22, Pages 8281-8295, ISSN 0021-9991, http://dx.doi.org/10.1016/j.jcp.2010.07.008.

[2] Dagan, G. (1989), *Flow and Transport in Porous Formations*, Springer, New York

[3] Fornberg B. and Flyer N. (2015). *Solving PDEs with radial basis functions*. Acta Numerica, 24, pp 215-258 doi:10.1017/S0962492914000130

[4] Kansa E.J. (1990), *Multiquadrics, a scattered data approximation scheme with applications to computational fluid dynamics. I. Surface approximations and partial derivatives estimates*, Comput. Math. Appl. 19, 127–145.

[5] Kansa E.J. (1990), *Multiquadrics, a scattered data approximation scheme with applications to computational fluid dynamics. II. Solutions to parabolic, hyperbolic and elliptic partial differential equations*, Comput. Math. Appl. 19, 147–161.

[6] Muskat, M. (1937), *The Flow of Homogeneous Fluids Through Porous Media*, McGraw-Hill, New York.

[7] Neuman, S. P., and P. A. Witherspoon (1969), *Theory of flow in a confined two aquifer system*, Water Resour. Res., 5, 803 – 814, doi:10.1029/WR005i004p00803.

[8] Severino G. (2011) - *Stochastic analysis of well-type flows in randomly heterogeneous porous formations*, Water Resources research, Volume 47, Issue 3, W03520, DOI: 10.1029/2010WR009840

[9] Severino G., Santini A. and Sommella A. (2008), *Steady flows driven by sources of random strength in heterogeneous aquifers with application to partially penetrating wells*, Stochastic Environmental Research and Risk Assessment, Volume 22, Issue 4, 567–582

[10] Smereka P. (2006) - *The Numerical Approximation of a Delta Function with Application to Level Set Methods*, Volume 211, Issue 1, Pages 77-90

Optimized Schwarz methods for a class of evolution problems

Giovanna Califano
Università degli Studi di Salerno
via Giovanni Paolo II, 132 84084 - Fisciano Italy
g.califano@unisa.it

Dajana Conte
Università degli Studi di Salerno
via Giovanni Paolo II, 132 84084 - Fisciano Italy
dajconte@unisa.it

In this talk we exhibit Schwarz Waveform Relaxation (WR) methods for fractional diffusion-wave equations of the form

$$\frac{\partial u}{\partial t}(x,t) - \frac{\nu}{\Gamma(\beta)} \int_0^t (t-\tau)^{\beta-1} \frac{\partial^2 u}{\partial x^2}(x,\tau) d\tau = f(x,t), \quad \beta \in (-1,1)$$

for $x \in \Omega \subseteq \mathbb{R}$ and $t > 0$, taken together with Dirichlet boundary conditions and with the initial condition $u(x,0) = u_0(x)$ for $x \in \Omega$.
Such equations describe anomalous diffusion processes and wave propagation in viscoelastic materials. They are interesting in the physical, chemical and engineering literature, as for example filtering to improve satellite image classification and to map burned areas, furthermore they are applied in image structure preserving denoising (see [1] and [2] and references therein contained). Other applications of the fractional diffusion equations deal with modeling anomalous heat transport in geothermal reservoirs (see [6]). Schwarz WR methods have been mainly developed and analysed for several kinds of PDEs [3, 4, 5], and consist in decomposing the spatial domain into subdomains (Domain decomposition technique) and solve iteratively time dependent problems on subdomains, exchanging information at the boundary. Domain decomposition methodology is well suited for parallelization on architectures such as GPUs or multicore CPUs. First of all we consider the classical Schwarz WR method on infinite spatial domain. If we decompose the domain into two subdomains it assumes the form

$$\begin{cases} \mathcal{L}(u_1^{k+1}) = f & in\ \Omega_1 \times \mathbb{R}_+ \\ u_1^{k+1}(L,t) = u_2^k(L,t) & t > 0 \\ u_1^{k+1}(x,0) = u_0(x) & x \in \Omega_1 \end{cases} \qquad \begin{cases} \mathcal{L}(u_2^{k+1}) = f & in\ \Omega_2 \times \mathbb{R}_+ \\ u_2^{k+1}(0,t) = u_1^k(0,t) & t > 0 \\ u_2^{k+1}(x,0) = u_0(x) & x \in \Omega_2 \end{cases}$$

where an initial guess $u_1^0(0,t)$ and $u_2^0(L,t)$, $t \in \mathbb{R}_+$, needs to be provided and where the operator $\mathcal{L}$ is defined from

$$\mathcal{L}(u) = u_t - \nu \partial^{-\beta} u_{xx}.$$

We observe as this method make use of Dirichlet transmission condition at the artificial interfaces. We analyse the convergence behaviour of the classical Schwarz WR method on infinite spatial domain. We first prove both the linear convergence rate on unbounded time intervals and the superlinear asymptotic convergence rate on bounded time intervals,

showing as Dirichlet boundary conditions at the artificial interfaces inhibit the information exchange between the subdomains and therefore slow down the convergence of the method. So, we construct optimal Schwarz WR methods both on infinite spatial domain and on finite spatial domain, by decomposing the spatial domain into N subdomains and by providing the transmission conditions which assure convergence in N iterations. The Optimal Schwarz WR method on 2 subdomains assume the form

$$\begin{cases} \mathcal{L}(u_1^{k+1}) = 0 & in\ \Omega_1 \times \mathbb{R}_+ \\ u_{1,x}^{k+1} + \Lambda^+(u_1^{k+1}) = u_{2,x}^k + \Lambda^+(u_2^k) & x = L,\ t > 0 \\ u_1^{k+1} = 0 & x \in \Omega_1,\ t = 0 \end{cases}$$

$$\begin{cases} \mathcal{L}(u_2^{k+1}) = 0 & in\ \Omega_2 \times \mathbb{R}_+ \\ u_{2,x}^{k+1} + \Lambda^-(u_2^{k+1}) = u_{1,x}^k + \Lambda^-(u_1^k) & x = 0,\ t > 0 \\ u_2^{k+1} = 0 & x \in \Omega_2,\ t = 0 \end{cases}$$

where Λ^+ and Λ^- are linear operators acting on the boundary in time and having corresponding symbols

$$\lambda^+ := +\frac{s^\gamma}{\sqrt{\nu}}, \lambda^- := -\frac{s^\gamma}{\sqrt{\nu}}.$$

The research that led to the present talk was partially supported by a grant of the group GNCS of INDAM.

References

[1] E. Cuesta, Ch. Lubich and C. Palencia, 2006 *Convolution quadrature time discretization of fractional diffusion-wave equations*, Math. Comp. 75, 673–696.

[2] E. Cuesta and C. Quintano, 2015 *Linear fractional-based filter as a pre-classifier to map burned areas in Mediterranean countries*, Int. J. Remote Sens. 36, 3293–3316.

[3] M.J.Gander and H.Zhao, 2002 *Overlapping Schwarz waveform relaxation for the heat equation in n dimensions*, BIT 42, 779–795.

[4] M.J.Gander, L. Halpern and F. Nataf, 2003 *Optimal Schwarz waveform relaxation for the one dimensional wave equation*, SIAM J. Numer. Anal. 41, 1643–1681.

[5] M.J.Gander and Ch. Rohde, 2005 *Overlapping Schwarz waveform relaxation for convection-dominated nonlinear conservation laws*, SIAM J. Sci. Comput. 27, 415–439.

[6] Y. Luchko and A. Punzi, 2011 *Modeling anomalous heat transport in geothermal reservoirs via fractional diffusion equations*, Int. J. Geomath. 1, 257–276.

Multidimensional Iterative Filtering method. A new way to decompose high–dimensional and non–stationary signals

Antonio Cicone
INdAM and Università degli Studi dell'Aquila
via Vetoio, 1 67100 - L'Aquila Italy
antonio.cicone@univaq.it

Haomin Zhou
Georgia Institute of Technology
686 Cherry St, 30332 - Atlanta, GA, USA
hmzhou@math.gatech.edu

Iterative Filtering, which is an alternative technique to the Empirical Mode Decomposition algorithm for the decomposition of non–stationary and non–linear signals, has been proved recently to be convergent for any L^2 signal [1]. In this talk we introduce its extension to higher dimensions, called Multidimensional Iterative Filtering algorithm, and we show the performance of this new technique when applied to the decomposition of syntectic and real life 2D signals.

References

[1] Cicone, Antonio and Liu, Jingfang and Zhou, Haomin 2016 *Adaptive Local Iterative Filtering for Signal Decomposition and Instantaneous Frequency analysis*. Applied and Computational Harmonic Analysis. doi:10.1016/j.acha.2016.03.001. ArXiv:1411.6051.

Some numerical error bounds for the log-ratio transformations in compositional data analysis

Antonio Maratea
Università degli studi di Napoli "Parthenope"
Centro Direzionale, Isola C4, 80143 - Napoli, Italy
antonio.maratea@uniparthenope.it

Ardelio Galletti
Università degli studi di Napoli "Parthenope"
Centro Direzionale, Isola C4, 80143 - Napoli, Italy
ardelio.galletti@uniparthenope.it

Data for which the relative abundance is more important than the absolute quantity are called *compositional* and arise in a number of fields, ranging from Geochemistry to Archaeology, Agriculture, Statistics, Economics and more. For such data, the information content to be extracted and analyzed is conveyed into the ratio of parts, instead of the absolute amount. A typical example is the chemical analysis of a rock sample: what matters are ratios of parts expressed in percentages or fractions, while the absolute weight of the parts is irrelevant. Another way for saying this is that the sample space should be scale invariant. Given the scale invariance, comparing samples of different weights requires them to be standardized to a common reference quantity (1 for unity, 100 for percentages, 10^6 for parts per million and so on), and the obvious way to obtain this standardization is to divide each sample by its total weight. This simple operation, called *closure*, subtly introduces a constraint on the data, which loose a degree of freedom, and hence causes a spurious correlation (the closure problem) that misleads following analysis. While the special nature of compositional data and some warnings on their handling have been formulated more than a century ago, it is no more than three decades that compositional data have found a proper representation and a complete formulation, mainly thanks to the seminal work of Aitchison [1] and the developments it solicited (see [3] for a compendium).
More formally, when N sample data are all positive, and it is meaningful to analyze them in terms of ratios, the vector

$$\mathbf{x_j} = [x_{j1}, \ldots, x_{jD}]$$

of strictly positive numbers expressing the D measured quantities on each sample $j \in \{1, \ldots, N\}$ in Euclidean space is called a *composition*. A desirable property of compositions is scale invariance, that is $\mathbf{x_j}$ and $\alpha\mathbf{x_j}$ should map to the same vector in the sample space $\forall\alpha \in \mathbb{R}^+$ and this can be obtained through the closure operator, defined as:

$$\mathcal{C}(\mathbf{x}) = \kappa \left[\frac{x_1}{\sum_{i=1}^{D} x_i}, \ldots, \frac{x_D}{\sum_{i=1}^{D} x_i} \right] \tag{1}$$

Once the closure operator is applied for standardization, the sample space becomes constrained, looses one degree of freedom and changes its nature: it is reduced to the D-dimensional simplex. The open D-dimensional simplex Δ^k, closed to $\kappa > 0$, is the set

of vectors having positive components with constant sum κ, that is:

$$S^D = \left\{ [x_1, \ldots, x_D] \mid x_i \in \mathbb{R}^+, \forall i \in \{1, \ldots, D\} \wedge \sum_{i=1}^{D} x_i = \kappa \right\}. \tag{2}$$

Notice that any vector $\mathbf{x}$, having D real positive components, can be always rescaled so that its components sum to a positive constant κ (usually 1 or 100) through closure. Once proper operations are introduced, the open simplex and the Euclidean space can be shown to be isomorphic. The *additive log-ratio* and the *centred log-ratio* transformations are two of the possible realizations of the isomorphism between the two vector spaces (the simplex and the Euclidean space). The additive log-ratio is the transformation $alr : S^D \to R^{D-1}$ defined as follows:

$$alr(\mathbf{x}) = \left[\log \frac{x_1}{x_D}, \ldots, \log \frac{x_{D-1}}{x_D} \right] \tag{3}$$

where the choice of the x_i at the denominator is arbitrary. Its inverse is:

$$alr^{-1}(\mathbf{y}) = \mathcal{C}\Big[e^{y_1}, \ldots, e^{y_{D-1}}, 1 \Big]. \tag{4}$$

The centred log-ratio is the transformation $clr : S^D \to U^D$, where U^D is an hyperplane in R^D, defined as follows:

$$clr(\mathbf{x}) = \left[\log \frac{x_1}{\mathrm{g}(\mathbf{x})}, \ldots, \log \frac{x_D}{\mathrm{g}(\mathbf{x})} \right] = \log \frac{\mathbf{x}}{\mathrm{g}(\mathbf{x})} \tag{5}$$

where $\mathrm{g}(\mathbf{x})$ is the geometric mean of the components of $\mathbf{x}$. Its inverse is:

$$clr^{-1}(\mathbf{y}) = \mathcal{C}\Big[e^{y_1}, \ldots, e^{y_D} \Big] = \mathcal{C}\Big(e^{\mathbf{y}} \Big). \tag{6}$$

Since both transformations include logarithms of ratios of parts, their computation accuracy is strongly affected by the closeness of the values (ratios close to one produce logarithms close to zero) and can generate not negligible distortions due to the unbounded propagation of the errors on the available data. Purpose of the study is to perform a sensitivity analysis and to reveal the compositions for which the transformations can, or cannot, be accurately computed: following the approach presented in [2], the error propagation in using both the *alr* and *clr* transformations will be studied; specifically, it will be shown that the amplification factors of the relative errors from the data $\mathbf{x}$ to the solutions $alr(\mathbf{x})$ and $clr(\mathbf{x})$ are, under some circumstances, unbounded and should hence be carefully managed. The practical consequence is that special care must be taken when operating on data that are in a certain area of the simplex where the transformations are component-wise ill conditioned.

References

[1] J Aitchison. *The Statistical Analysis of Compositional Data*. Chapman & Hall, Ltd., London, UK, UK, 1986.

[2] L. Damore, R. Campagna, A. Galletti, L. Marcellino, and A. Murli. A smoothing spline that approximates laplace transform functions only known on measurements on the real axis. *Inverse Problems*, 28(2), 2012.

[3] J. J. Egozcue and V. Pawlowsky. Simplicial geometry for compositional data. In *Compositional Data Analysis in the Geosciences: From Theory to Practice*, pages 67–77. Geological Society, Nov 2008.

On the employ of time series in the numerical treatment of differential equations

Martina Moccaldi
Department of Mathematics, University of Salerno
Via Giovanni Paolo II, 132 84084 - Fisciano (SA) Italy
mmoccaldi@unisa.it

Raffaele D'Ambrosio
Department of Mathematics, University of Salerno
rdambrosio@unisa.it

Beatrice Paternoster
Department of Mathematics, University of Salerno
beapat@unisa.it

Federico Rossi
Department of Chemistry and Biology, University of Salerno
frossi@unisa.it

In this talk, we present a numerical method that integrates differential equations by exploiting the a-priori known information about the qualitative behaviour of the exact solution. We focus on problems characterized by an oscillatory dynamics, for which time series of experimental data are also given and can be properly merged into the numerical scheme. Indeed, classical numerical methods could require a very small step-size to accurately follow the oscillations because they are constructed in order to be exact (within round-off error) on polynomials up to a certain degree. For this reason, we propose a method that is constructed in order to be exact on functions other than polynomials, following the well-known strategy of exponential fitting [4]. These basis functions are supposed to belong to a finite dimensional space (the so-called fitting space) and are properly chosen according to the behaviour of the exact solution. As a result, the coefficients of the corresponding numerical method are no longer constant as in the classical case, but are functions of a parameter characterizing the exact solution, whose value is clearly unknown. Hence, we need to deal with the two main problems deriving from exponential fitting technique: the choice of a suitable fitting space and the estimate or the computation of the parameter which the numerical method depends on.
We show how approaching these aspects by taking into account the existing theoretical studies on the problem and observing the time series of experimental data. Since we numerically integrate problems having periodic waves as fundamental solutions, we choose a trigonometrical fitting space, whose functions depend on a parameter which is the frequency of oscillations of the exact solution. We propose estimating the parameter by minimizing the leading term of the local discretization error [2]. However, when time series of experimental data are available, we can choose the frequency of observed oscillations as an estimate of the parameter, thus avoiding expensive procedures based on solving nonlinear systems of equations as in [1].

We focus on the oscillatory dynamics occurring in the well-known Belousov-Zhabotinsky reaction, that generally consists of the oxidation of an organic substance by bromate ions facilitated by a metal ion (cerium or iron) in an acid medium. In such reactions, oscillations are observed in the concentrations of the metal ion [5]. Chemical kinetics is described in the well-known Oregonator model developed by Fields-Köros-Noyes [3]. We numerically integrate this ODE system following the above-mentioned exponential fitting strategy. Since we observe oscillations in time series of experimental data [5], we use a trigonometrically fitted space and we choose the frequency of observed oscillations as an estimate of the parameter which the coefficients of the method depend on.
Numerical experiments will be provided to show that such an adapted method accurately follows the oscillations observed in experimental data, without strongly reducing the step-size as in the classical case. Moreover, the analysis of experimental data provides a cheap estimate of the parameter.
In summary, adapted methods may guarantee a better balance between accuracy and efficiency than classical ones but require the computation of the parameter. Therefore, applying the exponential fitting strategy is convenient only if the optimal parameter selection is not too expensive. This limit is overtaken when experimental data are available because the parameter can be estimated without increasing the computational cost at all.

The research that led to the present talk was partially supported by a grant of the group GNCS of INDAM.

References

[1] D'Ambrosio, R., Esposito, E. and Paternoster, B. 2012 *Parameter estimation in exponentially fitted hybrid methods for second order differential problems.* J. Math. Chem. 50, 155–168.

[2] D'Ambrosio, R., Moccaldi, M., Paternoster, B., *Parameter estimation in adapted numerical methods for reaction-diffusion problems*, J. Sci. Comput. (submitted)

[3] Epstein, I. R., Pojman, J. A. (1998) *An Introduction to Nonlinear Chemical Dynamics.* Oxford University Press. New York.

[4] Ixaru, L.Gr., Vanden Berghe, G. 2004 *Exponential Fitting.* Kluwer. Boston-Dordrecht-London.

[5] Rossi, F., Budroni, M. A., Marchettini, N., Cutietta L., Rustici, M. and Turco Liveri, M. L. 2009 *Chaotic dynamics in an unstirred ferroin catalyzed Belousov-Zhabotinsky reaction.* Chem. Phys. Lett. 480, 322–326.

Mathematical Models in Life Sciences - Part I

PROPOSERS

Marcello Delitala
Dip. di Scienze Matematiche, Politecnico di Torino
Corso Duca degli Abruzzi, 24 1029 - Torino Italy
marcello.delitala@polito.it

Marco Scianna
Politecnico di Torino
Corso Duca degli Abruzzi, 24 1029 - Torino Italy
marco.scianna@polito.it

SPEAKERS

Alberto M. Bersani
Dipartimento di Ingegneria Meccanica e Aerospaziale - Sapienza University
alberto.bersani@sbai.uniroma1.it

Chiara Giverso
MOX– Modellistica e Calcolo Scientifico. Dipartimento di Matematica "F. Brioschi", Politecnico di Milano, Milano,
chiara.giverso@polimi.it

Marco Scianna
Dip. di Scienze Matematiche, Politecnico di Torino
marco.scianna@polito.it

Elena Piretto
Dip. di Scienze Matematiche, Politecnico di Torino
elena.piretto@polito.it

Valerio Cusimano
Istituto di Analisi dei Sistemi ed Informatica "Antonio Ruberti", CNR Roma
valerio.cusimano@iasi.cnr.it

The presentations are in part related to the research activities of the participants to the SIMAI study group on Life and Environmental Sciences. They will show several mathematical models and results, both analytical and numerical, applied to many biological and collective systems in Life Sciences. These will span over a wide range of approaches, including continuum mechanics, reaction-diffusion equations, delay differential equations, inverse problems, optimal control, statistics, measure theory, population dynamics, and hybrid and multiscale methods.

A Mathematical Model of the Action of Stem Cells for Cardiac Tissue Regeneration

Alberto M. Bersani
Dipartimento di Ingegneria Meccanica e Aerospaziale - Sapienza University
via Eudossiana, 18 00184 - Roma Italy
alberto.bersani@sbai.uniroma1.it

Daniele Andreucci
Dipartimento di Scienze di Base e Applicate per l'Ingegneria - Sapienza University
via A. Scarpa, 16 00161 - Roma Italy
daniele.andreucci@sbai.uniroma1.it

Enrico Bersani
Laboratorio di Strutture e Materiali Intelligenti - Sapienza University
Palazzo Caetani, via San Pasquale snc, 04012 - Cisterna di Latina (LT) Italy
enrico.bersani@gmail.com

Ivan Giorgio
Department of Structural and Geotechnical Engineering, Sapienza University
via Eudossiana, 18 00184 - Roma Italy
International Research Center for the Mathematics and Mechanics of Complex Systems (MeMoCS), Italy
ivan.giorgio@uniroma1.it

Mario Ledda
Institute of Translational Pharmacology (IFT-CNR)
via Fosso del Cavaliere, 100 00133 - Roma Italy
mario.ledda@ift.cnr.it

Antonella Lisi
Institute of Translational Pharmacology (IFT-CNR)
via Fosso del Cavaliere, 100 00133 - Roma Italy
antonella.lisi@ift.cnr.it

Claudio De Lazzari
Institute of Clinical Physiology (IFC-CNR)
via S. Martino della Battaglia, 44 00185 - Roma Italy
claudio.delazzari@ifc.cnr.it

Stem cells have shown to have a high potential for the treatment of heart failure (infarct) through regeneration of cardiac tissue and restoration of cardiac contractility. In a previous paper [1] a first, simplified, numerical model of the action of stem cells was proposed with the aim of studying the optimal protocol for the stem implant in the tissue in order to replace the necrotic area (localization of the implant, number of stem cells to be implanted in each injection, implant times and so on).

The model described the cell growth, the nutrient transport and its consumption via reaction-diffusion equations. Since the stem tend to reconstruct the damaged tissue, substituting the necrotic cells, the shrinking of the ischemic area led to a moving boundary problem.
The theoretical and numerical model assumed, for simplicity, a spherical symmetry of the necrotic area. The stem cells distribution and their proliferation near the ischemic area, as well as the transport of nutrients were studied and were correlated with several parameters, as the maximum reaction rate, the saturation coefficient, the cell death parameter, the stem cell and the nutrient diffusion coefficient, the nutrient flux, the radius of the necrotic area, the implantation factor, the stem cell decay rate.
Several parameters were obtained from literature, while others were taken in physiologically reasonable ranges.
The research group from IFT-CNR recently performed several experiments in order to relate pH, stem cells growth, metabolism and mortality to the temperature, the glucose concentration and nutrient volume.
In this communication we test the previous model with the experimental data, in order to tune the parameters and give some preliminary, though still semiquantitative, predictions, also with a view to modify the geometry of the infarcted area.

References

[1] Andreucci, D., Bersani, A.M., Dell'Acqua, G., Bersani, E., De Lazzari, C., Ledda, M., Lisi, A. and Pontrelli, G. 2013 A Reaction-Diffusion Numerical Model to Predict Cardiac Tissues Regeneration Via Stem Cell Therapy. In *MASCOT11 Proceedings* (ed. R. M. Spitaleri). IMACS Series in Computational and Applied Mathematics, vol. 17, pp. 11-20, IMACS, Rome.

An interfacial growth model of tumor angiogenesis

Chiara Giverso
Dipartimento di Scienze Matematiche, Politecnico di Torino
Corso Duca degli Abruzzi, 24, 10129 - Torino Italy
chiara.giverso@polito.it

Pasquale Ciarletta
MOX - Dipartimento di Matematica, Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
pasquale.ciarletta@polimi.it

In order to sustain cancer growth beyond a critical size of about 1-2 mm, tumor cells can stimulate new vessels formation across distances of some millimeters, in a process called angiogenesis. The capability of cancer cell to promote angiogenesis mostly relies on the expression of a chemical factor, called vascular endothelial growth factor (VEGF), that induces endothelial cell proliferation and promotes their migration inside the extracellular space towards the source of the growth factor. The process of endothelial cells proliferation can be described by the interfacial growth theory [1], as it occurs in the endothelial layer of the capillary wall (190-270 nm), which is much smaller than the tumor-capillary distance (1-5 mm) and the capillary lumen (4-5 μm). Thus, we propose an original mechanistic approach to angiogenesis, defining a thermo-dynamically-consistent continuous model of interfacial growth that takes into account the creation of new endothelial cells at the interface between the pre-existing vasculature and the extracellular environment and the spatio-temporal evolution of the VEGF inside the domain [2]. In particular, the derived free-boundary mathematical model encapsulates i) the diffusion equation for the VEGF, ii) the interfacial mass, momentum and energy balance for the endothelial cells and iii) the volumetric mass, momentum and energy balance for the extracellular space and the capillary lumen. Finite element simulations have been performed on a 2D geometry, using the open-source program FreeFem++, and they show that both the morphology and the dynamics of the sprouting vessels are controlled by the bulk diffusion of VEGF and the chemo-mechanical and geometric properties at the capillary interface. Furthermore, the predicted morphologies resulting from the numerical simulations strikingly resemble the tree-like vascular structures experimentally observed in vivo and in vitro. Thus, we suggest that the emergence of tree-like vessel structures during tumour angiogenesis may result from the free boundary instability driven by competition between chemical and mechanical phenomena occurring at different length-scales.

References

[1] Ciarletta P., Preziosi L. and Maugin G.A. 2013 *Mechanobiology of interfacial growth.* J. Mechan. Phys. Solids, 61: 852-872.

[2] Giverso C. and Ciarletta P. 2016 *Tumour angiogenesis as a chemo-mechanical surface instability.* Sci. Rep., 6: 22610.

Coherent Modelling Switch between Pointwise and Distributed Representations of Cell Aggregates

Marco Scianna
Politecnico di Torino
Corso Duca degli Abruzzi, 24 10129 - Torino Italy
marco.scianna@polito.it

Biological systems are typically formed by different cell phenotypes, characterized by specific biophysical properties and behaviors. Moreover, cells are able to undergo differentiation or phenotypic transitions upon internal or external stimuli. In order to take these phenomena into account, we here present a modelling framework in which cells can be described either as pointwise/ concentrated particles or as distributed masses, according to their biological determinants. A set of suitable rules then defines a coherent procedure to switch between the two mathematical representations. The theoretical environment describing cell transition can be then enriched by including cell migratory dynamics and duplication/apoptotic processes, as well as the kinetics of selected diffusing chemicals influencing the system evolution. Finally, biologically relevant numerical realizations are presented in this talk: in particular, they deal with the growth of a tumor spheroid and with the initial differentiation stages of the formation of the zebrafish posterior lateral line. Both phenomena mainly rely on cell phenotypic transition and differentiated behaviour, thereby constituting biological systems particularly suitable to assess the advantages of the proposed model.

References

[1] Colombi, A., Scianna, M., Preziosi, L. 2016. *Coherent modelling switch between pointwise and distributed representations of cell aggregates*. Submitted.

Cancer, immune system and therapies: an evolutionary arms race

Elena Piretto
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
elena.piretto@polito.it

Marcello Delitala
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
marcello.delitala@polito.it

Mario Ferraro
Università degli Studi di Torino
Via Pietro Giuria, 1 10125 - Torino Italy
ferraro@ph.unito.it

The need to suppress cancer has involved the evolution of powerful control mechanisms and a complex immune system to allow the development of animals with large bodies and long lives. On the other hand, however, different tumor types have arisen exhibiting resistance to the immune system and, nowadays, therapy. In the history of life, then, immune system and cancer have been engaged in an evolutionary arms race driven by the twin forces of mutation and selection. Ideally therapies should be a resolutive weapon, but, despite great progresses during the last 50 years or so, the race still goes on.

The aim of this talk is to present a mathematical model, as *in silico* laboratory, providing some indication on the effectiveness of therapies. In the framework of ecology of cancer, we focus on two cancer subpopulation competing for resources and with immune system cells. The model is analytically and computationally studied to elucidate its properties and emerging behaviors.

First we consider an *in vitro* system, i.e. the cancer clones in absence of the immune cells, with an additional pressure of two types of therapies: chemotherapy and antiangiogenic therapy. The results are in good agreement with some well known experimental data obtained under laboratory conditions. The analysis suggests that if the selective pressure is low under no-treatment conditions, then therapies, increasing the selective pressure, are usually beneficial. On the contrary if a medical treatment is applied to a system with high internal selective pressure adverse effects may result, due to the enhancement of selection.

In vivo a much richer variety of behaviors appears, due to the interactions with the immune system; for instance for strong intertumoral competition, and high recognition levels by the immune system, stable stationary states are replaced by sustained oscillations. Results confirms the critical importance of the overall selective pressure to define effective therapies.

In conclusion this model supports the idea, nowadays prevalent in the biomedical literature, that an effective combination therapy can be designed using more conventional treatments together with immunotherapy.

Closed-loop control of tumor growth by means of anti-angiogenic administration

Valerio Cusimano
Istituto di Analisi dei Sistemi ed Informatica A. Ruberti, IASI-CNR
Via dei Taurini 19, 00185 Roma, Italy
valerio.cusimano@iasi.cnr.it

Pasquale Palumbo
Istituto di Analisi dei Sistemi ed Informatica A. Ruberti, IASI-CNR
Via dei Taurini 19, 00185 Roma, Italy
pasquale.palumbo@iasi.cnr.it

Federico Papa
Istituto di Analisi dei Sistemi ed Informatica A. Ruberti, IASI-CNR
Via dei Taurini 19, 00185 Roma, Italy
federico.papa@iasi.cnr.it

Anti-angiogenic therapies are relatively new cancer treatments, proposed at first by Folkman [2] in the early seventies, consolidated along the nineties by several discoveries on the main principles regulating tumor angiogenesis [6] and widely debated in several theoretical and experimental studies throughout the last decade. Anti-angiogenic treatments aim at inhibiting the development of the vascular network necessary to support tumor growth during the vascular phase, so providing a way to control the heterogeneous and growth-unconstrained tumor population throughout the control of the homogeneous and growth-constrained population of endothelial cells.
In this work, we investigate and design a closed-loop model-based control law based on anti-angiogenic administration. This study is based on a quantitative model describing the growth of experimental tumors under the control of the vascular network. The adopted model was proposed by Hahnfeld et all. in [3], where the authors introduced the concept of the carrying capacity of the vasculature, i.e. the tumor volume potentially sustainable by the vasculature. The paper represents one of the first attempts to model, with a minimal number of parameters, the interplay between the dynamics of the tumor volume and of the carrying capacity, with or without administration of anti-angiogenic drugs.
The design of the closed-loop makes use of the feedback linearization [1]. The regulator is synthesized as a feedback from the state and a nonlinear observer is used to estimate the state of the system since only the tumor volume is directly measurable. The closed-loop control formally aims to track a desired low level of tumor volume. The control scheme allows to set independently the control and the observer parameters thanks to the special structural properties of the model that guarantee the separability of estimation and feedback control algorithms.
To demonstrate the validity of the algorithm, simulations are performed setting the model parameters and the initial conditions to the values estimated in [3]. Such an estimation was based on experimental data of Lewis lung carcinoma implanted in C57BL/6 mice. The data referred to volume measurements of both untreated control tumors and treated

tumors under a regimen with endostatin. For the observer initialization, the initial condition of the tumor volume was set equal to the measurement of the tumor volume at day zero while the carrying capacity is allowed to vary in the percentage range of $[-40, +200]\%$ with respect to real value. For each pair of initial conditions, two different targets have been address that is:

1. to keep the final value of the tumor volume within 10% of variation of the reference level;

2. to keep the average daily amount of the administered drug within 40% of variation with respect to the value assumed in [3].

Numerical simulations revealed to be extremely promising, showing a noticeable level of robustness against a wide range of the observer initial conditions and of the carrying capacity actual values.

References

[1] Cusimano, V. and Palumbo, P. and Papa, F. 2015 *Closed-loop control of tumor growth by means of anti-angiogenic administration* IEEE Conference on Decision and Control (CDC), pp. 7789–7794

[2] Folkman, J. 1972 *Anti-Angiogenesis: New Concept for Therapy of Solid Tumors.* Annals of Surgery, vol. 175, pp. 409–416.

[3] Hahnfeldt, P. and Panigrahy D. and Folkman J. and Hlatky L. 1999 *Tumor Development under Angiogenic Signaling: A Dynamical Theory of Tumor Growth, Treatment Response, and Postvascular Dormancy.* Cancer Research, vol. 59, pp. 4770–4775.

[4] Kerbel, R. S. 1991 *Inhibition of Tumor Angiogenesis as a Strategy to Circumvent Acquired Resistance to Anti-cancer Therapeutic Agents.* BioEssays, vol. 13, pp. 31–36.

[5] Kerbel, R. S. 1997 *A Cancer Therapy Resistant to Resistance.* Nature, vol. 390, pp. 335–336.

[6] Klagsbrun, M. and Soker, S. 1993 *VEiGF/VPF: the Angiogenesis Factor Found?.* Current Biology, vol. 3, pp. 699–702.

Mathematical Models in Life Sciences - Part II

PROPOSERS

Marcello Delitala
Dip. di Scienze Matematiche, Politecnico di Torino
Corso Duca degli Abruzzi, 24 1029 - Torino Italy
marcello.delitala@polito.it

Marco Scianna
Politecnico di Torino
Corso Duca degli Abruzzi, 24 1029 - Torino Italy
marco.scianna@polito.it

SPEAKERS

Armando Bazzani
Dipartimento di Fisica e Astronomia, Università di Bologna
armando.bazzani@unibo.it

Paolo Freguglia
Dip. di Matematica Pura e Applicata, Università dell'Aquila
pfreguglia@gmail.com

Alberto M. Bersani
Dipartimento di Ingegneria Meccanica e Aerospaziale - Sapienza University
alberto.bersani@sbai.uniroma1.it

Barbara Coluzzi
Dip. Me. Mo. Mat., Università La Sapienza di Roma
barbara.coluzzi@sbai.uniroma1.it

Pierluigi Vellucci
Dip. Me. Mo. Mat., Università La Sapienza di Roma
pierluigi.vellucci@sbai.uniroma1.it

The presentations are in part related to the research activities of the participants to the SIMAI study group on Life and Environmental Sciences. They will show several mathematical models and results, both analytical and numerical, applied to many biological and collective systems in Life Sciences. These will span over a wide range of approaches, including continuum mechanics, reaction-diffusion equations, delay differential equations, inverse problems, optimal control, statistics, measure theory, population dynamics, and hybrid and multiscale methods.

Self-organized properties in activity fluctuations of neural networks

Armando Bazzani
Dipartimento di Fisica e Astronomia, Università di Bologna
via Irnerio 46, 40126 - Bologna Italy
armando.bazzani@unibo.it

Paolo Freguglia
Dipartimento di Ingegneria e Scienze dell'Informazione e Matematica, Università de L'Aquila
via Vetoio (Coppito 1), 67100 - Coppito (L'Aquila) Italy
pfreguglia@gmail.com

Elena Tea Russo
Dipartimento di Fisica e Astronomia, Università di Bologna
via Irnerio 46, 40126 - Bologna Italy
elenatea.russo@gmail.com

The study of Complex Systems has shown as the interaction structure among the elementary components plays a more essential role in defining the macroscopic properties than the nature itself of the considered components[1]. The application of network theory to analyzed the big data bases of biological and social systems has shed light on the topological and statistical properties of the interaction networks that characterize the complexity feature. However, the mere statistical analysis of data is not able to understand the correlation of the microscopic dynamics of the elementary components and the network structure and may induce erroneous explanations of the individual behavior at the base of empirical observations. The recent possibility of collecting dynamical big data bases on Complex Systems has pointed out the necessity of developing new theoretical approaches to study the evolution of complex systems as dynamical systems on a network structure. In this framework, we consider the problem as a very small perturbation of a Complex System may change the macroscopic state of the system itself. This phenomenon may be particularly relevant in neural systems that can be considered a paradigmatic example of Complex Systems. In particular we study the activity fluctuation properties of Integrate and Fire (IF) networks[2, 3, 4] connected by a graph that represent the synaptic connections, under the effect of an external stimulus. It has been shown that with this model it is easy that neurons synchronize, i.e. that close neurons fire consequentially in a small time interval. Our aim is to study the existence of a self-organized dynamical states characterized by a fat tail fluctuation distributions of the neural activity if the input strength overcome a certain threshold[5, 6]. Even if the studied graphs are very simple, the model is complex enough to present a substantial number of these critical events. A small random stimulus can generate notably large fluctuations in the activity of the network: these peaks of activity are interpreted as avalanches of inter-neural signals, especially if the system is on the edge of equilibrium. To tackle complex system's modeling it is possible to take advantage from Stochastic Dynamical Systems theory (discrete Markov Chains)[7] and the self-criticality theory[8]. These models introduce

an effective description of the microscopic dynamics and of the microscopic interactions by means of the Master equation, whose properties can be numerically and analytically studied. We illustrate our results on simple example of IF neural networks[9].

References

[1] Newman M. 'Network: an introduction' Oxford University Press. (2010).

[2] Rafael D. Vilela and Benjamin Lindner 'Comparative study of different integrate-and-fire neurons: Spontaneous activity, dynamical response, and stimulus-induced correlation' Phys. Rev. E 80, 031909 (2009).

[3] A. N. Burkitt 'A review of the integrate-and-fire neuron model: I. Homogeneous synaptic input' Biol Cybern 95: 1–19 (2006).

[4] A. N. Burkitt 'A review of the integrate-and-fire neuron model: II. Inhomogeneous synaptic input and network properties' Biol Cybern 95:97–112 (2006).

[5] J Hesse, T. Gross, Self-organized criticality as a fundamental property of neural systems. Front Syst Neurosci, 2014 Sep 23;8:166. doi: 10.3389/fnsys.2014.00166. (2014).

[6] C.J. Perez, A. Corral, A.D. Guilera, K.Christensen, A. Arenas 'On the Self-Organized Criticality and Synchronization in Lattice Models of Coupled Dynamical Systems' Int. J. Mod. Phys. 10, Nos. 8 & 9, 1-41. (1996).

[7] L. Arnold Random dynamical systems, Springer Monographs in Mathematics, Springer. (2003).

[8] Matthias Rybarsch and Stefan Bornholdt 'Self-organized criticality in neural network models' in Criticality in Neural Systems (eds D. Plenz and E. Niebur), Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, Germany. doi: 10.1002/9783527651009.ch10, (2014).

[9] Felix Droste, Anne-Ly Do Thilo Gross 'Analytical investigation of self-organized criticality in neural networks' J R Soc Interface. 6;10(78): 20120558 (2013).

Dynamical of network structures: application to biological processes

Paolo Freguglia
Dipartimento di Ingegneria e Scienze dell'Informazione e Matematica, Università de L'Aquila
via Vetoio (Coppito 1), 67100 - Coppito (L'Aquila) Italy
pfreguglia@gmail.com

Armando Bazzani
Dipartimento di Fisica e Astronomia, Università di Bologna
via Irnerio 46, 40126 - Bologna Italy
armando.bazzani@unibo.it

Elena Tea Russo
Dipartimento di Fisica e Astronomia, Università di Bologna
via Irnerio 46, 40126 - Bologna Italy

Network structures have been recognized as one of the most suitable mathematical tools to model the interactions among the elementary components of complex systems. These interactions allow to introduce a dynamics in the network structure that may suggest the existence of critical phenomena in evolution of biological systems. The models can be applied to describe the dynamics of genetic networks, neural networks and ecological networks. In particular we discuss some statistical properties of Markov models associated to dynamical systems on graphs, which are support of biological networks, by considering the effects of the nonlinear interactions among connected nodes on the macroscopic stationary states of the network. However the study of evolutionary mathematical models which take into account all the possible biological scales, from the genome scale up to the ecological scale is far to be realized. There are still very useful 'mesoscopic' models where one neglect the details of the biochemical interactions at genetic or protein level, but tries to describe the effect of biological networks at the phenotype level of individuals. In the paper[1] we have proposed a description for the evolutionary Darwinian behaviour of an individual as standard representative M of a species, according to an ago-antagonist approach[2]. In the original formulation, this approach considers two counteracting actions related to the possible expression of a new phenotype: the agonist action promotes the expression of the new phenotypes, whereas the antagonist action tends to maintain the old one. Under the effect of random mutations and/or of the selective pressure due to the external environment one of the two action prevails and the new phenotype is expressed or the old phenotype is fixed in the population. From a mathematical point of view, the ago-antagonist model represents the evolution process as transition from an initial neutral equilibrium state towards new equilibria induced by a random perturbation. The proposed model joins three concepts that are at the base of just as many assumptions to model evolutionary systems. At first one assumes that networks are suitable to represent the interaction structures among different genes whose global activity (or inactivity) can be related to the expression (or non-expression) of a new phenotype by the individuals of a population. Certainly this idea is supported by

the success of network theory to give an overall view of empirical genetic data[3, 4]. The network structure not only define a concept of neighbour that is more general than the topological concept[5], but allows to point out key nodes that could play a fundamental role in determining the evolution of the systems (controllability problem [6]). Recently dynamical genetic data are recorded so that one should have the possibility of performing a study to validate this assumption. The second hypothesis concerns the existence of an ago-antagonist mechanism at the base of gene activity. This mechanism describes the genetic dynamics during an evolutionary process as an irreversible transition from an initial neutral state (that is in principle quasi-stationary, but with very long stability time) toward the fixation of an active (agonist) or inactive (antagonist) state. Of course we do not have an explanation at biochemical level of such a mechanism and this assumption can be interpreted as a simple effective description of complex underlying dynamics, which is consistent with empirical observations at mesoscopic scale. The last assumption is that the evolution of genetic networks depends on the link weights that measure the interaction among the genes by means of a control parameter (the paroxysmal parameter) in the ago-antagonist model. This hypothesis characterizes the evolutionary dynamics as the result of a sequence of mutations (for example, related to the activation of certain genes), that can trigger a cascade effect to induce a n irreversible macroscopic transition on the whole network. The consequent dynamics is interpreted in term of a self-organized criticality since the macroscopic state of the network can remain in a neutral condition up to when the mutation of some key genes triggers the cascade effect, whose propagation depends on both the network structure and the previous history. Our model gives a mesoscopic description of an evolutionary process whose validity has to be studied from empirical observations on specific cases where one has information of the genetic networks involved[7]. We finally remark that the main features of the model are:

1. the existence of a threshold effect for the random environmental pressure to trigger an evolution process with the possibility of long time steady states;

2. the irreversibility of the evolution process and its critical dependence on specific events (mutation) and on its past history (self-organized criticality);

3. the existence of different time scale for evolution that could explain the discontinuity in the evolution processes;

4. the complex character of the phenotype with the possibility of considering phenotype interaction by means of a hierarchical structure of genetic networks (multiplex theory[8]).

References

[1] Bazzani A., Freguglia P., "Ago-Antagonist Theory in Darwinian Evolutuion", *Theoretical Biological Forum*, 1 – 2: 25-35, (2013)

[2] Cherruault Y., *Modèles et methods mathématiques pour les sciences du vivant*, PUF, Paris, 1998

[3] Van Someren E.P., Wessels L.F., Backer E., Reinders M.J. "Genetic network modeling", *Pharmacogenomics*, (4):507-25 (2002).

[4] Somogyi R. Carol Ann Sniegoski C.A. *Modeling the complexity of genetic networks: Understanding multigenic and pleiotropic regulation Complexity* , Volume 1, Issue 6: 45–63, (1996).

[5] Scheffer M. et al. "Anticipating Critical Transitions", *Scienc* 338-6105: 344-348 (2012).

[6] Scheffer M., "Carpenter S.R. "Catastrophic regime shifts in ecosystems: linking theory to observation TRENDS", *Ecology and Evolution*, 18-12, 648 (2003).

[7] Stadler B.M., Stadler P.F., Wagner G.P., "Fontana W. The topology of the possible: formal spaces underlying patterns of evolutionary change". *J. Theor Biol.*, Nov 21;213(2):241-74 (2001)

[8] Yang-Yu Liu Y.Y, Slotine J.J., Barabási A.L. "Controllability of complex networks", *Nature* 473, 167–173 (2011)

Modelling miRNA intracellular regulation activity

Alberto M. Bersani
Dipartimento di Ingegneria Meccanica e Aerospaziale - Sapienza University
via Eudossiana, 18 00184 - Roma Italy
alberto.bersani@sbai.uniroma1.it

Enrico Bersani
Laboratorio di Strutture e Materiali Intelligenti - Sapienza University
Palazzo Caetani, via San Pasquale snc, 04012 - Cisterna di Latina (LT) Italy
enrico.bersani@gmail.com

Pierluigi Vellucci
Dipartimento di Scienze di Base e Applicate per l'Ingegneria - Sapienza University
via Antonio Scarpa, 16 00161 - Roma Italy
pierluigi.vellucci@sbai.uniroma1.it

MicroRNAs (miRNAs) are small non coding RNA molecules, composed of about twenty nucleotides, targeting specific portions of RNA messenger (mRNA) molecules, reducing their stability and enhancing translation repression [7, 10]. Since about one third of human mRNA is targeted by miRNA and a single miRNA species can target over one hundred molecules, miRNA have emerged as powerful regulators of intracellular reactions and can be considered as potential drug targets to indirectly regulate sensible proteins like oncogenes or tumor suppressors in cancer [1, 10] or to regulate cell proliferation [2] and in particular stem cell proliferation and differentiation [6, 7].
We can list two broad classes of models:

a) miRNA biogenesis (i.e., the simulation of the intricate phases of miRNA transcription, maturation, RISC detection and cytoplasmic transport);

b) mature miRNA dynamics within the intracellular environment (in particular the interaction with cytoplasmic protein networks), simulating the interaction with mRNA involved in network homeostasis.

At the best of our knowledge, the most detailed models of miRNA activity were described in [3, 8, 9], mostly based on the mass action principle.
In this communication we focus on a model of the second class, where dynamics is regulated by three basic molecular species: free mature miRNA, miRNA-target mRNA complex, mRNA, and a fourth species, the encoded protein. The dynamics is a first order one, the "speed" of a reaction being described by a first order ordinary nonlinear differential equation using mass action law.
Such models are quite general and can be applied, like "modules", at any mRNA in the network, since miRNA dynamics is in some sense universal.
In particular, our interest is in the application of the three-species miRNA model to the intracellular network regulating osteosarcoma cell behavior; we focus our attention on phospholipases, a family of enzymes overlooked in this kind of models.
Specificity of phospholipases in cell types has been recently appreciated and investigated.

Our aim is to study the kinetics of such enzymes within intracellular networks, modulated by miRNA action, to discover molecular targets to approach osteosarcoma therapy.
In these models it is crucial to determine the kinetic constants by means of a process of Reverse Engineering, using the experimental data concerning the concentration of mRNA in the cell (see, for example, [4, 5]).

References

[1] Aguda B.D., Kima Y., Piper-Hunter M.G., Friedman A. and Marsh C.B. 2008 *MicroRNA regulation of a cancer network: Consequences of the feedback loops involving miR-17-92, E2F, and Myc*. PNAS 105, 19678–19683.

[2] Bueno M.J., Pérez de Castro I. and Malumbres M. 2008 *Control of cell proliferation pathways by microRNAs*. Cell Cycle 20, 3143–3148.

[3] Levine E., Jacob E.B. and Levine H. 2007 *Target-Specific and Global Effectors in Gene Regulation by MicroRNA*. Biophys. J. 93, L52–L54.

[4] Lo Vasco V.R., Leopizzi M., Puggioni C. and Della Rocca C. 2014 *Ezrin silencing remodulates the expression of Phosphoinositide-specific Phospholipase C ensymes in human osteosarcoma cell lines*. J. Cell Commun. Signal. 8, 219–229.

[5] Lo Vasco V.R., Leopizzi M. and Della Rocca C. 2015 *Ezrin-related Phosphoinositide pathway modifies RhoA and Rac1 in human osteosarcoma cell lines*. J. Cell Commun. Signal. 9, 55–62.

[6] Porrello E.R. 2013 *microRNAs in cardiac development and regeneration*. Clin. Sc. 125, 151–166.

[7] Shenoy A. and Blelloch R.H. 2014 *Regulation of microRNA function in somatic stem cell proliferation and differentiation*. Nat. Rev. Mol. Cell Biol. 15, 565–576.

[8] Wang X., Li Y., Xu X. and Wang Y.H. 2010 *Toward a system-level understanding of microRNA pathway via mathematical modeling*. Biosystems 100, 31-38.

[9] Xue X., Xia W. and Wenzhong H. 2013 *A modeled dynamic regulatory network of NF-κB and IL-6 mediated by miRNA*. Biosystems 114, 214–218.

[10] Zhang J., Yu X.H., Yan Y.G., Wang C. and Wang W.J. 2015 *PI3K/Akt signaling in osteosarcoma*. Clin. Chim. Acta 444, 182–192.

An alternative, Renormalization Group based, approach to Michaelis-Menten kinetics

Barbara Coluzzi
Dipartimento di Scienze di Base ed Applicate per l'Ingegneria, *Sapienza* University
via A. Scarpa, 14, 00161 - Roma, Italy
barbara.coluzzi@sbai.uniroma1.it

Alberto M. Bersani
Dipartimento di Ingegneria Meccanica ed Aerospaziale, *Sapienza* University
via Eudossiana, 18 00184 - Roma, Italy
alberto.bersani@sbai.uniroma1.it

Enrico Bersani
Laboratorio di Strutture e Materiali Intelligenti, *Sapienza* University
Palazzo Caetani, via San Pasquale s.n.c., 04012 Cisterna di Latina, Latina, Italy
enrico.bersani@gmail.com

The Michaelis-Menten kinetics [4] is a well known successful example of mathematical application to life science. Both the standard quasi-steady-state approximation (sQSSA) and the total one (tQSSA) are essential starting points for the analysis of data on enzymatic reactions, the latter being appropriate for a larger set of parameter values [1]. Indeed, these approximations should be more rigorously regarded as the zeroth order results of perturbation expansions that involve solving systems of both singularly and regularly perturbed differential equations [1, 3].

Here, against the background of the standard perturbation expansion for Michaelis-Menten kinetics beyond the sQSSA, with the usual choice of the expansion parameter $\varepsilon = e_0/s_0$ (where e_0 is the initial enzyme concentration and s_0 is the initial substrate one), we present our main results on the application to this dynamical system of the alternative approach to singularly perturbed differential equations proposed by Chen, Goldenfeld and Oono [2], that is based on the renormalization group framework (SPDERG). In fact, the Michaelis-Menten kinetics is an example of boundary layer problem, that already turned out to be particularly demanding for the application of the presently considered method [5].

By directly renormalizing the bare adimensionalized initial values, we are able to recover the standard results up to the known first order, while contemporaneously calculating the contributions to the inner solutions up to the second order, for the first time to our knowledge. Noticeably, the differential equation to be solved for the obtention of the first order outer complex contribution is simpler within the present approach. Moreover, despite of the cumbersome but not in principle difficult calculations, we verify that one gets in fact the uniform solution, hence the best approximation to the original problem one, without the need to apply matching conditions or to remove terms that otherwise would appear twice. In conclusion, we present the main results of an accurate mathematical analysis of the SPDERG in the case of Michaelis-Menten kinetics, that show both the advantages and the limits of the method in the present case. The work suggests first of

all further applications within the same context, in particular to the more experimentally interesting case in which one takes the tQSSA as starting point, and it could also be perhaps useful for more formal and concise developments of the approach.

References

[1] Bersani, A.M., Bersani, E., Dell'Acqua, G. and Pedersen, M.G. 2015, *Continuum Mech. Thermodyn.* **27**, 659.

[2] L.-Y. Chen, N. Goldenfeld and Y. Oono, 1994, *Phys. Rev. Lett.* **73**, 1311; 1996, *Phys. Rev. E* **54**, 376.

[3] Mascia, C. and Montefusco, E. 2014 *Un Invito alla Biomatematica*, (Edizioni La Dotta, Bologna).

[4] Michaelis, L. and Menten, M.L. 1913 *Biochem. Z.* **49**, 333; English review and translation in Johnson, K.A. and Goody, R.S., 2011 *Biochemistry* **50**, 8264.

[5] E. Raccah, *Applicazione delle tecniche del gruppo di rinormalizzazione alle cinetiche enzimatiche*, Tesi di Laurea Specialistica in Fisica, Sapienza University of Rome, Italy (A.A. 2011/2012).

Tihonov approach for multidimensional systems in bio-informatics

Pierluigi Vellucci
Dipartimento di Scienze di Base e Applicate per l'Ingegneria, Sapienza University
Via Antonio Scarpa n. 16, 00161 Roma
pierluigi.vellucci@sbai.uniroma1.it

Alberto M. Bersani
Dipartimento di Ingegneria Meccanica e Aerospaziale, Sapienza University
Via Eudossiana n. 18, 00184 Roma
alberto.bersani@sbai.uniroma1.it

Alessandro Borri
Istituto di Analisi dei Sistemi ed Informatica "Antonio Ruberti" (IASI-CNR)
Piazzale A. Moro, 7 00185 Roma - Italy
alessandro.borri@iasi.cnr.it

Alessandro Milanesi
Dipartimento di Scienze di Base e Applicate per l'Ingegneria, Sapienza University
Via Antonio Scarpa n. 16, 00161 Roma
alessandro.milanesi@sbai.uniroma1.it

Let us consider an enzyme, E, which reacts with a protein, X, resulting in an intermediate complex, C. In turn, this complex can break down into a product, X_p, and the enzyme E. It is frequently assumed that formation of C is reversible while its breakup is not. The process is represented by the following sequence of reactions

$$X + E \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} C \xrightarrow{k_2} X_p + E. \tag{1}$$

Following [4], as reported in [1], we have the adimensionalized initial value problem:

$$\begin{aligned} \frac{du}{d\tau} &= -u + (u + \kappa - \lambda)v, \qquad && u(0) = 1, \\ \epsilon\frac{dv}{d\tau} &= u - (u + \kappa)v, && v(0) = 0, \end{aligned} \tag{2}$$

where E_T, X_T are respectively the initial concentrations of the enzyme E and of the protein X, and $\tau = k_1 E_T t$, $u(\tau) = \frac{X(t)}{X_T}$, $v(\tau) = \frac{C(t)}{E_T}$, $\lambda = \frac{k_2}{k_1 X_T}$, $\kappa = \frac{k_2 + k_{-1}}{k_1 X_T} = \frac{k_m}{X_T}$ and $\epsilon = \frac{E_T}{X_T}$. This is the Heineken-Tsuchiya-Aris system, [4]. Origin $(u, v) = (0, 0)$ is the unique fixed point of (2). Let $\tau = \epsilon s$. Equations (2) can be rewritten in the equivalent form

$$\begin{aligned} \frac{du}{ds} &= \epsilon\varphi(u, v), \\ \frac{dv}{ds} &= u - (u + \kappa)v \end{aligned} \tag{3}$$

where $\varphi(u,v) = -u + (u+\kappa-\lambda)v$. Operating the substitution $w := u - \kappa v$, i.e., $v = \frac{u-w}{\kappa}$, we obtain: $\varphi(u,w) = -u + (u+\kappa-\lambda)\frac{u-w}{\kappa}$ and $\frac{dw}{ds} = \epsilon\varphi(u,w) + u(u-w) - \kappa w$. Following [9], the way we will handle parametrized systems consists of including the parameter ϵ as a new dependent variable as in (4). This merely acts to augment the matrix A by adding a new center direction that has no dynamics. In this way, equation (3) becomes

$$\begin{aligned} \frac{du}{ds} &= \epsilon\varphi(u,w), \\ \frac{dw}{ds} &= -\kappa w + u(u-w) + \epsilon\varphi(u,w), \\ \frac{d\epsilon}{ds} &= 0 \end{aligned} \tag{4}$$

The eigenvalues are given by 0 (multiplicity 2) and $-\kappa$. To find a center manifold, we search for a function $h(u,\varepsilon)$ such that

$$D_u h(u,\epsilon)\,(0 + f(u,h(u,\epsilon),\epsilon)) + \kappa h(u,\epsilon) - g(u,h(u,\epsilon),\epsilon) = 0 \tag{5}$$

where

$$\begin{aligned} f(u,h(u,\epsilon),\epsilon) &= \epsilon\varphi\left(u,h(u,\epsilon)\right), \\ g(u,h(u,\epsilon),\epsilon) &= u\left(u - h(u,\epsilon)\right) + \epsilon\varphi\left(u,h(u,\epsilon)\right). \end{aligned} \tag{6}$$

We assume

$$h(u,\epsilon) = a_1u^2 + a_2u\epsilon + a_3\epsilon^2 + \dots \tag{7}$$

Substituting (7) into (5), and truncating to second order terms, we obtain: $(ka_1 - 1)\,u^2 + \left(ka_2 + \frac{\lambda}{\kappa}\right)u\epsilon + \kappa a_3\epsilon^2 + \dots = 0$. Equating terms of the same power to zero gives $a_1 = \frac{1}{\kappa}$, $a_2 = -\frac{\lambda}{\kappa^2}$ and $a_3 = 0$. Hence, the center manifold for system (4) is:

$$h(u,\epsilon) = \frac{1}{\kappa}u^2 - \frac{\lambda}{\kappa^2}u\epsilon + \dots \tag{8}$$

which, for $\kappa = 1$, gives the result shown in ([3], p.8, example 3), where the author uses equations

$$\begin{aligned} \frac{du}{d\tau} &= -u + (u+c)v, \\ \epsilon\frac{dv}{d\tau} &= u - (u+1)v. \end{aligned} \tag{9}$$

By applying the sQSSA (which corresponds to impose $\epsilon = 0$), we have

$$\begin{aligned} \frac{du}{d\tau} &= -\frac{\lambda u}{\kappa+u}, \\ v &= \frac{u}{\kappa+u}. \end{aligned} \tag{10}$$

We observe that the center manifold (8) is asymptotically sufficiently close to (10). In fact, since $v = \frac{u-w}{\kappa}$ from (8), and $w = h(u,\epsilon) = \frac{1}{\kappa}u^2 - \frac{\lambda}{\kappa^2}u\epsilon + \dots$, we have $v = \frac{u}{\kappa}\left(1 - \frac{w}{u}\right) = \frac{u}{\kappa}\left(1 - \frac{1}{\kappa}u + \frac{\lambda}{\kappa^2}\epsilon + \dots\right)$. Since equation (10) is obtained putting $\epsilon = 0$, one has

$$v \sim \frac{u}{\kappa}\left(1 - \frac{u}{\kappa}\right) \sim \frac{u}{\kappa}\left(\frac{1}{1+\frac{u}{\kappa}}\right), \quad \text{for } u \to 0 \tag{11}$$

which is the second equation of (10). We can conclude that, supposing $\epsilon \ll 1$, the center manifold determined in this way approximates the solution given by sQSSA.
The sQSSA is related to Tihonov's Theorem [5]-[7]. Let x be a scalar and $\mathbf{y}$ be a two-dimensional vector, i.e. $\mathbf{y} = (y_1, y_2)^t$. All variables are real, and ϵ is positive. Tihonov's Theorem ensures that, under certain conditions, the solution $x(t,\epsilon)$, $\mathbf{y}(t,\epsilon)$ of the full initial value problem

$$\begin{aligned} \frac{dx}{dt} &= f(x,\mathbf{y}) \\ \epsilon\frac{d\mathbf{y}}{dt} &= \mathbf{g}(x,\mathbf{y}), \end{aligned} \tag{12}$$

$$x = \alpha, \quad \mathbf{y} = \boldsymbol{\beta}, \quad \text{for } t = 0 \tag{13}$$

is connected with the solution $x_0(t)$, $\mathbf{y}_0(t) = \boldsymbol{\phi}(x_0(t))$ of the reduced problem

$$\begin{aligned} \frac{dx}{dt} &= f(x,\boldsymbol{\phi}(x)) \\ \mathbf{y} &= \boldsymbol{\phi}(x), \end{aligned} \tag{14}$$

$$x = \alpha, \quad \text{for } t = 0 \tag{15}$$

by the limit relations

$$\begin{aligned} &\lim_{\epsilon\to 0} x(t,\epsilon) = x_0(t), \qquad 0 \le t \le T_0 \\ &\lim_{\epsilon\to 0} \mathbf{y}(t,\epsilon) = \mathbf{y}_0(t) = \boldsymbol{\phi}(x_0(t)) \quad 0 < t \le T_0 \end{aligned} \tag{16}$$

for some number T_0. For the total QSSA in Enzyme Kinetics, Tihonov's Theorem is related to the Theory of Center Manifold [9] in a way enlightened in a paper in preparation [2]. Introducing the new variables $\bar{X} = X + C$ and $u = \frac{\bar{X}}{X_T}$, $v = \frac{C}{E_T}$, we obtain the center manifold

$$v = \frac{u}{\eta+\kappa_m}\left(1 - \frac{w}{u}\right) = \frac{u}{\eta+\kappa_m}\left(1 - \frac{\sigma\kappa_m}{(\eta+\kappa_m)^2}u + \frac{1}{(\eta+\kappa_m)^2}\epsilon + \dots\right),$$

which, again, is asymptotically sufficiently close to the tQSSA solution

$$v = \frac{\eta + \kappa_m + \sigma u - \sqrt{(\eta+\kappa_m+\sigma u)^2 - 4\eta\sigma u}}{2\eta\sigma}.$$

Tihonov's papers [5]-[7], [8] contain a significant further generalization. It deals with differential systems of the form

$$\begin{aligned} \frac{dx}{dt} &= f(x, y_1, \dots, y_m; t), \\ \epsilon_j \frac{dy_j}{dt} &= g_j(x, y_1, \dots, y_m; t), \qquad j = 1, 2, \dots, m, \end{aligned} \tag{17}$$

where $\epsilon_1, \dots, \epsilon_m$ are parameters that depend on each other in such a way that $\epsilon_1 \to 0$ implies

$$\frac{\epsilon_{j+1}}{\epsilon_j} \to 0, \qquad j = 1, 2, \dots, m-1. \tag{18}$$

The y_j and x are vectors of arbitrary dimensions. The aim of the talk is to apply this result to n-state biological systems as, for example, the well-known Goldbeter-Koshland cycle and the double phosphorylation mechanism in a tQSSA framework.

References

[1] A.M. Bersani, E. Bersani, G. Dell'Acqua, M.G. Pedersen, New trends and perspectives in nonlinear intracellular dynamics: one century from Michaelis-Menten paper, Continuum Mechanics and Thermodynamics, 1-26, (2014).

[2] A.M. Bersani, E. Bersani, A. Borri, P. Vellucci, Dynamical aspects of the total QSSA in Enzyme Kinetics, in preparation.

[3] J. Carr, Applications of Center Manifold Theory. Springer-Verlag: New York, Heidelberg, Berlin (1981).

[4] F. G. Heineken, H. M. Tsuchiya, R. Aris, On the mathematical status of the pseudo-steady state hypothesis of biochemical kinetics, Mathematical Biosciences 1.1, 95-113, (1967).

[5] A.N. Tihonov, On the dependence of the solutions of differential equations on a small parameter. Matematicheskii Sbornik 64.2 (1948): 193-204.

[6] A.N. Tihonov, On a system of differential equations containing parameters. Matematicheskii Sbornik, 27 (1950), pp. 147-156.

[7] A.N. Tihonov, Systems of differential equations containing small parameters in the derivatives, Matematicheskii Sbornik 73.3 (1952): 575-586.

[8] W. Wasow, Asymptotic expansions for ordinary differential equations. Courier Corporation, 2002.

[9] S. Wiggins, Introduction to applied nonlinear dynamical systems and chaos. Vol. 2. Springer Science & Business Media, 2003.

Mathematical Models in Life Sciences - Part III

PROPOSERS

Marcello Delitala
Dip. di Scienze Matematiche, Politecnico di Torino
Corso Duca degli Abruzzi, 24 1029 - Torino Italy
marcello.delitala@polito.it

Marco Scianna
Politecnico di Torino
Corso Duca degli Abruzzi, 24 1029 - Torino Italy
marco.scianna@polito.it

SPEAKERS

Federico Papa
Istituto di Analisi dei Sistemi ed Informatica "Antonio Ruberti", CNR Roma
federico.papa@iasi.cnr.it

Alessandra Micheletti
Dip. Matematica, Università di Milano
alessandra.micheletti@unimi.it

Daniela Morale
Dip. Matematica, Università di Milano
daniela.morale@unimi.it

Camillo Cammarota
Dip. di Matematica, Università La Sapienza di Roma
cammar@mat.uniroma1.it

Maria Clara Nucci
Dip. di Matematica e Informatica, Università di Perugia
mariaclara.nucci@unipg.it

The presentations are in part related to the research activities of the participants to the SIMAI study group on Life and Environmental Sciences. They will show several mathematical models and results, both analytical and numerical, applied to many biological and collective systems in Life Sciences. These will span over a wide range of approaches, including continuum mechanics, reaction-diffusion equations, delay differential equations, inverse problems, optimal control, statistics, measure theory, population dynamics, and hybrid and multiscale methods.

A simple model of HIV epidemic in Italy: the role of the anti-retroviral treatment.

Federico Papa
Istituto di Analisi dei Sistemi ed Informatica 'A. Ruberti' - CNR
Via dei Taurini, 19 00185 - Roma Italy
federico.papa@iasi.cnr.it

Francesca Binda
Dipartimento di Scienze Biomediche e Cliniche 'L. Sacco', Università degli Studi di Milano
Via G. B. Grassi, 74 20157 - Milano Italy
francesca.binda@unimi.it

Marco Franzetti
Dipartimento di Scienze Biomediche e Cliniche 'L. Sacco', Università degli Studi di Milano
Via G. B. Grassi, 74 20157 - Milano Italy
marco.franzetti@unimi.it

Giovanni Felici
Istituto di Analisi dei Sistemi ed Informatica 'A. Ruberti' - CNR
Via dei Taurini, 19 00185 - Roma Italy
giovanni.felici@iasi.cnr.it

Alberto Gandolfi
Istituto di Analisi dei Sistemi ed Informatica 'A. Ruberti' - CNR
Via dei Taurini, 19 00185 - Roma Italy
alberto.gandolfi@iasi.cnr.it

Carmela Sinisgalli
Istituto di Analisi dei Sistemi ed Informatica 'A. Ruberti' - CNR
Via dei Taurini, 19 00185 - Roma Italy
carmela.sinisgalli@iasi.cnr.it

Claudia Balotta
Dipartimento di Scienze Biomediche e Cliniche 'L. Sacco', Università degli Studi di Milano
Via G. B. Grassi, 74 20157 - Milano Italy
claudia.balotta@unimi.it

We propose a simple ODE model to describe the evolution of HIV epidemic in Italy [2]. The model considers a single population of susceptibles, without distinction of high-risk groups within the general population, and accounts for the effects of immigration on both the general demography and the dynamics of the infected subpopulations. To represent the intra-host disease progression, the untreated infected population is distributed over four compartments in cascade according to the CD4 counts. A further compartment is added to represent infected people under anti-retroviral therapy. Treatment can be initiated at any stage of the disease progression with different per capita rates. Exit from

the treatment is allowed, followed by the return in the disease progression group.
Analytical results about model properties in its time-invariant form are provided, in particular the global stability of the equilibrium points is established either in the absence and in the presence of infected among immigrants.
The model parameters have been assessed on the basis of *a priori* knowledge coming from the literature and by means of best fitting of epidemiological and demographic data from official sources: the Italian Operative AIDS Center (COA) of the National Institute of Health (ISS) [1] and the National Institute for Statistics (ISTAT) [3]. The data concern the number of total infected, treated patients, new cases of AIDS and deaths from AIDS, over the decade 2003 div 2013.
The best fitting of the available data suggests that, in the 2003 div 2013 period, the per capita treatment rate of AIDS patients was the largest (0.0032 1/day), followed by the rate of patients with CD4 count between 350 and 200 cells/μl (0.0023 1/day). Early treatment with higher CD4 counts resulted negligible. With the parameter values so assessed, the epidemic evolution (taken as a reference evolution) was predicted until year 2025.
To assess the impact of different treatment strategies, we explored different scenarios by changing the per capita treatment rates. Assuming that all patients, irrespective of their CD4 count, could be eligible for treatment (with a per capita treatment rate equal to the maximal estimated value in 2003 div 2013), the model predicted a significant impact over AIDS incidence and mortality at year 2025 (43% reduction in both new cases of AIDS and number of AIDS deaths compared to the values of the reference evolution). Moreover, the model forecasted also a relevant decrease in the number of newly infected individuals (69% decrease), thus suggesting a benefit of early treatment strategy for the control of HIV infection.
The model is intended as an initial step towards a more complex model for the evolution of anti-retroviral drug resistance, in which, following the approach outlined in [4], susceptible individuals can be infected by different virus strains resistant to different drug classes, and mutations can occur during treatment.

References

[1] Camoni, L., Regine, V., Stanecki, K., et al. 2014 *Estimates of the number of people living with HIV in Italy*. Biomed. Res. Int. 2014, 1–6.

[2] Papa, F., Binda, F., Felici, G., Franzetti, M., Gandolfi, A., Sinisgalli, C., Balotta, C. *A simple model of HIV epidemic in Italy: the role of the anti-retroviral treatment*. Submitted to Math. Biosc. and Eng.

[3] Patruno, V., Venturi, M. and Roberto, S. *Intercensal population estimates. Demographic balance*. National Institute of Statistics of Italy (ISTAT). http://demo.istat.it/index.html

[4] Smith, R. J., Okano, J. T., Kahn, J. S., Bodine, E. N. and Blower, S. 2010 *Evolutionary Dynamics of Complex Networks of HIV Drug-Resistant Strains: The Case of San Francisco*. Science 327, 697–701.

Survival analysis and generalized linear models applied to the identification of risk factors in influenza-like epidemics

Alessandra Micheletti
Università degli Studi di Milano
Dip. di Matematica, via Saldini, 50 20133 - Milano Italy
alessandra.micheletti@unimi.it

Vittoria Colizza
Inserm & Universite Pierre et Marie Curie
Site Hopital St Antoine, 27 rue Chaligny, 75012 - Paris France
vittoria.colizza@inserm.fr

Francesca Ieva
Università degli Studi di Milano
Dip. di Matematica, via Saldini, 50 20133 - Milano Italy
francesca.ieva@unimi.it

In recent literature some mathematical and computational models have been developed in order to study the diffusion of an influenza epidemic, or more precisely influenza-like-illness (ILI) [1, 2, 4]. They came out to be very useful in 2009, during the alert announced by World Health Organization to prevent and control the pandemic due to a new strain of H1N1 virus. Also without serious alerts, every year during the flu epidemic peak, in almost all the European countries we assist to an increasing number of hospitalizations of people at risk (like children and elder patients), with a consequent increase of the costs covered by National Health Services and with a worrying decrease of the availability of beds and cares in hospitals. Thus, predicting models of the influenza diffusion might provide an effective help in programming and organizing the health resources necessary for the rescue. The aim of our study is the analysis of risk factors in a flu epidemic, on the basis of a sample of self-reported cases of ILI, provided by volunteers registered at the web sites of InfluenzaNet (http://www.influenzanet.eu) in the 2012-2013 season. The data where collected in seven different European countries. We modelled the occurrences of ILI cases as a non-homogeneous counting process, and we studied the influence of different factors both by applying logistic regression and by comparing the survival functions for different levels of the factors. Because of the strong non-homogeneity of the sample both in different countries and in different age classes, we stratified the sample and applied weighted general linear models to perform the logistic regression, and a weighted version of the Kaplan-Meier parameters estimators to identify the survival functions. Different weights have been chosen for different strata of the sample, according to differences put in evidence in previous studies [3].

References

[1] P Bajardi, C Poletto, J.J Ramasco, M Tizzoni, V Colizza, A Vespignani Human mobility networks, travel restrictions, and the global spread of 2009 H1N1 pandemic, *PLoS ONE* 6(1), e16591 (2011)

[2] D Balcan, B Gonçalves, H Hu, V Colizza, J.J Ramasco, A Vespignani Modeling the spatial spread of infectious diseases: the GLobal Epidemic and Mobility computational model, *Journal of Computational Science* 1, 132 (2010)

[3] P.Cantarelli, M. Debin, C. Turbelin, C. Poletto, T. Blanchon, A. Falchi, T. Hanslik, I. Bonmarin, D. Levy-Bruhl, A. Micheletti, D. Paolotti, A. Vespignani, J. Edmunds, K. Eames, R. Smallenburg, C. Koppeschaar, A. O Franco, V. Faustino, A.S. Carnahan, M. Rehn, V. Colizza, The representativeness of a European multi-center network for influenza-like-illness participatory surveillance, *BMC Medical Research Methodology*, Sep 20;14(1):984 (2014)

[4] W. Van den Broeck, M. Tizzoni, P. Bajardi, C. Poletto, J.J. Ramasco, D. Balcan, B. Goncalves, N. Perra, V. Colizza, A Vespignani, Real-time numerical forecast of global epidemic spreading: case study of 2009 A/H1N1 pdm, *BMC Medicine* 10 (2012), 165.

Stochastic modelling and simulation for ion channels

Daniela Morale
Università degli Studi di Milano
via Cesare saldini, 50 20133 - Milano Italy
daniela.morale@unimi.it

Ion channels are of major interest and form an area of intensive research in the fields of biophysics and medicine since they control many vital physiological functions.
We present a fully stochastic and discrete model describing the main characteristics of a multiple channel system. The movement of the ions is coupled, as usual, with a Poisson equation for the electrical field; we have considered, in addition, the influence of exclusion forces.
On the other hand, we discuss the nondimensionalization of the stochastic system by using real physical parameters, all supported by numerical simulations.
The specific features of both cases of micro- and nanochannels have been taken in due consideration with particular attention to the latter case in order to show that it is necessary to consider a discrete and stochastic model for ions movement inside the channels.
Possible open problems are discussed.

References

[1] D. Morale, M. Zanella, V. Capasso, W. Jaeger, Stochastic Modeling and Simulation of Ion Transport through Channels, Multiscale, Multiscale Modeling and Simulation, 14(1), 113–137, 2016

Amplitude Change in R and T Waves of Electrocardiogram during Exercise

Camillo Cammarota
Università degli Studi di Roma La Sapienza
Piazzale A. Moro 5 - 00185 Roma - Italy
cammar@mat.uniroma1.it

Mario Curione
Università degli Studi di Roma La Sapienza
Piazzale A. Moro 5 - 00185 Roma - Italy
mario.curione@uniroma1.it

The electrocardiogram (ECG) recorded during the exercise test is used to evaluate the presence of myocardial ischaemia [4]. During the test the patient on a bicycle ergometer is subjected to a workload increasing in time. The exercise is stopped when the heart rate reaches a maximum (acme), usually 85% of the estimated top heart rate based on the patient's age. After achieving peak workload the patient spends some minutes at rest until its heart rate recovers its basic value. The R and T waves of the ECG (fig.1) occur respectively at the end of the ventricular diastolic phase and at the end of the systolic phase, which are the times of maximum and minimum ventricular filling. The instantaneous heart rate is measured from the time intervals occurring between two consecutive R peaks, the RR intervals. The series of the RR intervals, of the R and T waves amplitudes extracted from the ECG of 65 healthy subjects during exercise are in fig. 2. The data are affected by large inter individual variability, due to amplitude variations across the subjects that affect proportionally the amplitudes of the R and T waves. Since we are interested in relative variation of these variables during time, we normalise each series dividing by its temporal mean. The mathematical model of the rescaled R and T series is

$$Y_i(t) = \mu(t) + Z_i(t),\ i = 1, ..., n;\ t = 1, ..., m \tag{1}$$

where i is the index of the subject, $\mu(t)$ is the population profile and the $Z_i(t)$'s are i.i.d. random variables with zero mean for each t and i and Var $Z_i(t) = \sigma_i(t)^2$. The $Z_i(t)$'s account for individual deviations from the population mean.

Data registration Data registration is an operation required in order to align prominent features. We use the landmark registration based on the fact that each RR series has a global minimum (acme), occurring at beat number, say t_i^*. Data registration of R and T series is performed putting the time of this common feature into a common value. This is accomplished extracting a window of $m = 600$ beats centred at t_i^* in each series, in such a way that the acme occurs at beat number 300. In the sequel we restrict the analysis to this window. Fig. 2 provides a representation of the data in this window.

Reduction of dimensionality and smoothing The basic operation for functional data is the reduction of dimensionality, that in our case is of the order of 10^3, the number of time observations. This can be done choosing an orthonormal set that spans a suitable

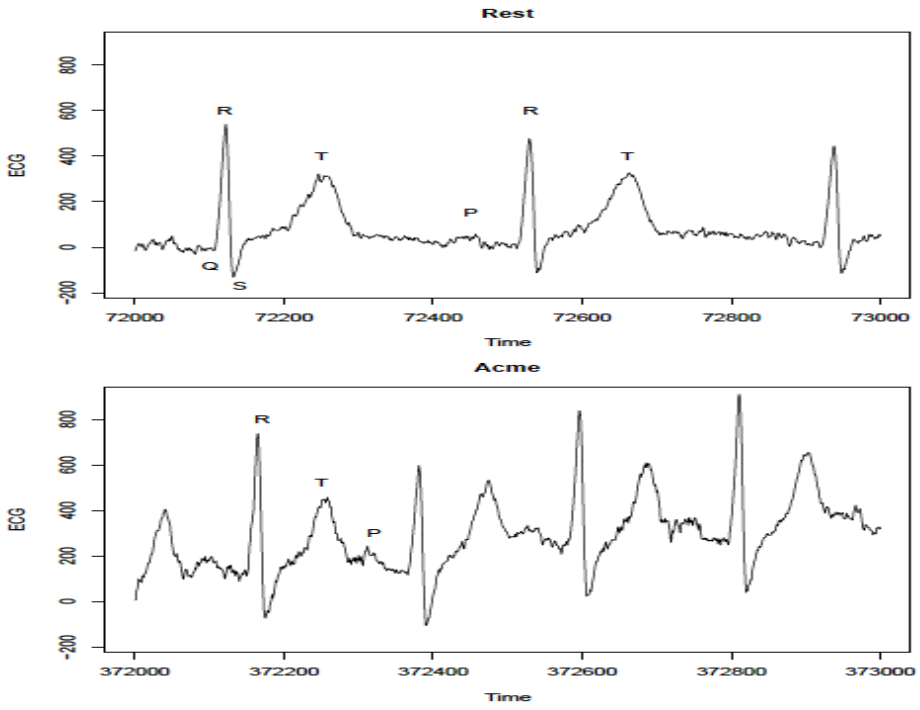


Figure 1: The exercise ECG of a normal subject at rest (top) and at acme (bottom)

functions subspace and projecting on this subspace. We use a set of cubic polynomials B-splines $\psi_k(t)$, $k = 1, ..., K$ with K of the order of 100. Since these are smooth functions, the reduction of dimensionality produces a smoothing of the series. Each function $X_i(t)$ can be replaced by its smoothed version $X_i^{(s)}(t)$, according to $X_i^{(s)}(t) = \sum_{k=1}^{K} c_{i,k}\ \psi_k(t)$ where the $c_{i,k}$ are suitable coefficients.

Pointwise confidence band An estimator for the population mean $\mu(t)$ is

$$\hat{\mu}(t) = \frac{1}{n}\sum_{i=1}^{n} X_i^{(s)}(t) \tag{2}$$

It is usual to consider two different types of confidence bands for the population mean: the pointwise and the simultaneous one. The pointwise confidence band can be obtained from the estimator of the variance of $Z(t)$:

$$\hat{\sigma}(t)^2 = \frac{1}{n-1}\sum_{i=1}^{n}(X_i^{(s)}(t) - \hat{\mu}(t))^2 \tag{3}$$

Then the pointwise confidence band for $\mu(t)$ of level $1-\alpha$ is

$$\hat{\mu}(t) \pm \hat{\sigma}(t)\ z_{1-\alpha/2}\ n^{-1/2} \tag{4}$$

where $z_{1-\alpha/2}$ is the standard normal quantile.

Simultaneous confidence band The simultaneous confidence band depends on the estimate of the correlation matrix C of $Z(t)$ obtained from the smoothed data. Usually

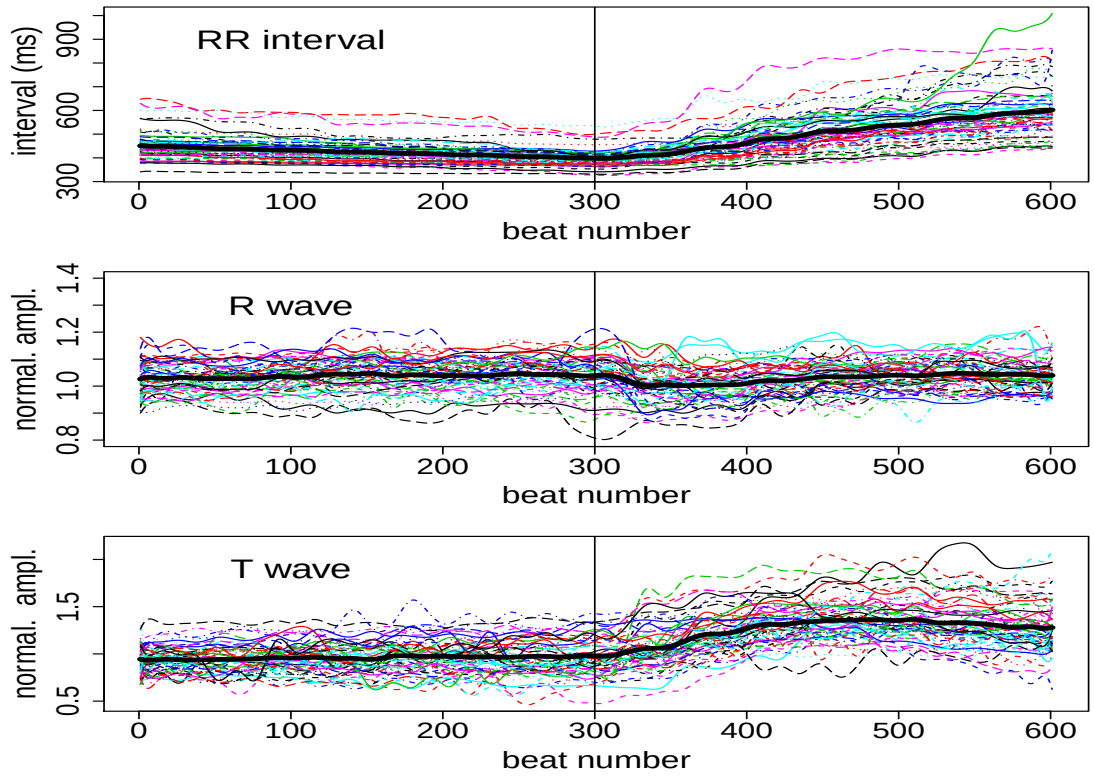


Figure 2: Time-mean rescaled and aligned series of a group of 65 normal subjects and their population mean (thick black line) of RR interval (top), R amplitude (centre) and T amplitude (bottom) during the exercise test. The vertical line denotes the acme. The series are restricted to a window of 600 beats centred at the acme. Adimensional units on vertical axis. Color on line.

one assumes that $Z(t)$ is a normal process with zero mean and covariance C and considers the random variable

$$M = \max_{t=1,\dots,m} \frac{|Z(t)|}{\sigma(t)} \tag{5}$$

The distribution of M can be obtained from simulations of the process $Z(t)$. Denoting $M_{1-\alpha}$ the quantile, the simultaneous confidence band of level $1-\alpha$ is [3]

$$\hat{\mu}(t) \pm \hat{\sigma}(t)\ M_{1-\alpha}\ n^{-1/2} \tag{6}$$

In fig. 3 the straight line of height 1 is not included in the band of the T wave so we conclude that the bump of T wave amplitude is significant.

SiZer In this approach the dataset is modeled using a single equation

$$\overline{Y}(t) = \mu(t) + \overline{Z}(t), \quad t = 1, ..., m$$

where $\overline{Y}(t)$ is the population mean obtained taking the mean over the subjects in eq. 1, and $\overline{Z}(t)$ is obtained in a similar way. In order to construct a confidence band for $\mu(t)$ we use the `R` package `SiZer` [5, 6]. This package performs a locally weighted polynomial regression centred at each point $t_j,\ j = 1, ..., k$ of a grid, a suitable subset of the time values. The weight is

$$w_j(t) = K((t - t_j)/h) / \sum_t K((t - t_j)/h)$$

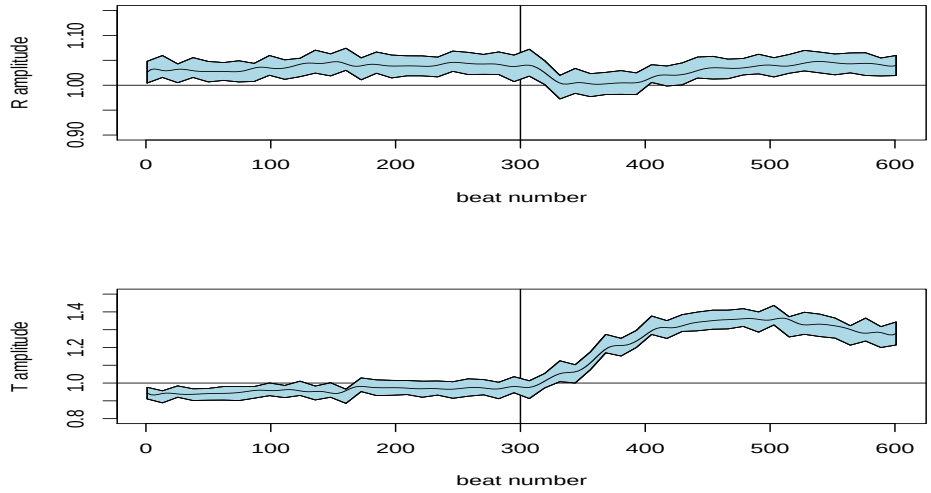


Figure 3: The simultaneous confidence band of 95% level of R and T amplitude.

where K is a Gaussian kernel, and h is the bandwidth. We use a second order polynomial

$$P_j(t) = \beta_0^{(j)} + \beta_1^{(j)}(t - t_j) + \beta_2^{(j)}(t - t_j)^2$$

and the parameters $\beta_0^{(j)}, \beta_1^{(j)}, \beta_2^{(j)}$ are estimated minimizing for any j the quantity $\sum_t (\overline{Y}(t) - P_j(t))^2 w_j(t)$ The value of h acts as a smoothing parameter. The theory of multivariate linear models provide both an estimate and a confidence interval for the polynomial coefficients $\beta^{(j)}$. The coefficients of zeroth order $\beta_0^{(j)}, j = 1, ..., k$ provide an estimator of the level; similarly the coefficients of first order $\beta_1^{(j)}$ provide an estimator of the derivative. The 95% confidence band for the population mean $\mu(t)$ allows to conclude that the two main features of the population mean of R and T series, i.e. the dip of R and the bump of T, occurring just after the acme (fig. 2), are significant.

These results [1] extend the previous one obtained by the authors on the R amplitude [2]. Amplitude changes of R and T waves seem to reflect the changes of electrical resistivity due to the number of red cells in the left ventricular chamber. Opposite trends in R and T wave amplitude after the acme present a specular behavior according to the Frank-Starling law.

References

[1] Cammarota and Curione (2016) *arXiv:1602.05907.*

[2] Curione, Cammarota et al. (2008) *Archives of medical science* **4** 51–56.

[3] Degras (2011) Simultaneous confidence bands for non parametric regression with functional data. *Statistica Sinica* 21: 1735–1765.

[4] Gibbons and Balady (2002) *J. Am. Coll. Cardiol.* **40** 1531 – 1540.

[5] R Development Core Team (2008) *R: A Language and Environment for Statistical Computing.*

[6] Sonderegger (2011) *SiZer: Significant Zero Crossings.* http://CRAN.R-project.org

Symmetries, Lagrangians, and conservation laws of biological systems

Maria Clara Nucci
Università degli Studi di Perugia
Dipartimento di Matematica e Informatica, 06123 Perugia (Italy)
nucci@unipg.it

In a review to honor the 50th Anniversary Year of the Journal of Theoretical Biology one reads: *It is frequently claimed that – like Newton's invention of calculus – biological theory will require 'new mathematics'.... There are, however, many areas of mathematics that have been neglected by theoretical biology that could prove to be of great value. Einstein's work on general relativity, for instance, made good use of mathematical ideas, in particular differential geometry that had previously been developed with completely different motivation. More likely than not, the formal structures have been set forth in some context, and await their discovery and subsequent development in representing biological theory* [4].
Since many mathematical tools used in Physics have also been used in biology with alternate success, we present a somewhat forgotten and neglected tool, a tool that in one of its outcomes, Noether symmetries, helped Einstein and Klein in their quarrel with Hilbert about the energy-momentum conservation of general relativity theory [9]. This tool is Lie continuous symmetries, that yield conservation laws, calculus of variation setting, and ultimately quantization.
The application of Lie symmetries to various biological models have already been shown to either provide more accurate predictions [5] or implement [1], [3], [6] the usual techniques related to qualitative and numerical analysis, that are common tools for any mathematical biologist.
We would like to stir up some controversy with the purpose of making both mathematicians and biologists pondering over some missed opportunities [2].
Since a good example is the best sermon, classical known mathematical models such as the Volterra-Verhulst-Pearl equation [10], [11] will be used to show the many symmetries they possess, the many Lagrangians and therefore different variational problems they admit [8], [7], and the conservation laws they lead to.
In the wake of Volterra's last papers [10], [11], examples of biological mathematical models given in terms of first-order ordinary differential equations that can be transformed into second-order Lagrangian systems will be also provided.

References

[1] Edwards, M. and Nucci, M.C. 2006 *Application of Lie group analysis to a core group model for sexually transmitted diseases*. J. Nonlinear Math. Phys. 13, 211–230.

[2] Freeman, J.D. 1972 *Missed opportunities*. Bull. Amer. Math. Soc. 78, 635–652.

[3] Gradassi, A. and Nucci, M.C. 2007 *Hidden linearity in systems for competition with evolution in ecology and finance*. J. Math. Anal. Appl. 333, 274–294.

[4] Krakauer, D.C. et al 2011 *The challenges and scope of theoretical biology.* J. Theor. Biol. 276, 269–276.

[5] Nucci, M.C. 2004 *Using Lie symmetries in epidemiology.* Electron. J. Diff. Eqns., Conference 12, 87–101.

[6] Nucci, M.C. and Leach, P.G.L. 2007 *Lie integrable cases of the simplified multistrain/two-stream model for tuberculosis and Dengue fever.* J. Math. Anal. Appl. 333, 430–449.

[7] Nucci, M.C. and Sanchini, G. 2015 *Symmetries, Lagrangians and Conservation Laws of an Easter Island Population Model.* Symmetry 7, 1613–1632.

[8] Nucci, M.C. and Tamizhmani, K.M. 2012 *Lagrangians for biological models.* J. Nonlinear Math. Phys. 19, 1250021.

[9] Rowe, D 2001 *Einstein meets Hilbert: At the Crossroads of Physics and Mathematics.* Phys. Perspect. 3, 379–424.

[10] Volterra, V. 1938 *Population growth, equilibria, and extinction under specified breeding conditions: a development and extension of the theory of the logisitc curve.* Human Biology 10, 1–11.

[11] Volterra, V. 1939 *Calculus of Variations and the Logistic Curve.* Human Biology 11, 173–178.

Computational Methods for Inverse Problems and Applications

PROPOSERS

Claudio Estatico
Dipartimento di Matematica, Università di Genova
via Dodecaneso, 35, 16146 - Genova Italy
estatico@dima.unige.it

Giuseppe Rodriguez
Dipartimento di Matematica e Informatica, Università di Cagliari
Viale Merello, 92, 09123 - Cagliari Italy
rodriguez@unica.it

SPEAKERS

Davide Bianchi
Dip. Scienza e Alta Tec., Univ. dell'Insubria, Como
ismaele.grimm@gmail.com

Patricia Díaz de Alba
Dip. di Mat. e Inf., Univ. di Cagliari
patricia.diazdealba@gmail.com

Caterina Fenu
Dip. di Informatica, Univ. di Pisa
kate.fenu@gmail.com

Silvia Noschese
Dip. di Matematica, Univ. di Roma "La Sapienza"
noschese@mat.uniroma1.it

Serena Morigi
Dip. di Matematica, Univ. di Bologna
serena.morigi@unibo.it

Emanuele Tavanti
Dip. di Ingegneria DITEN, Univ. di Genova
emanuele.tavanti@gmail.com

Inverse problems constitute one of the most important class of applied mathematical problems. They are ubiquitous in real world applications, from civil engineering to industrial and biomedical applications. They arise whenever it is necessary to estimate by indirect measurements physical parameters that cannot be directly observed. Important examples of technological processes based on inverse problems are computerized tomography, digital image deblurring, spaceborne remote sensing, non-destructive civil and geophysical prospection.

Recently, regularization theory has been extended to include new Tikhonov-like functionals or different functional spaces, all conceived in order to overcome some drawbacks of conventional approaches, such as oversmoothness and low sparsity of the regularized solution. At the same time, nonlinear models have been developed to reproduce with higher accuracy the behaviour of important physical systems. The challenge is to enhance important features of the true scene without loosing regularization and noise filtering capabilities. This aim can be pursued by both a better analytical study of the mathematical model of the real life scenario and an improvement of the inversion algorithms. In this respect, variational approaches in new functional spaces, effective heuristic methods for estimating the regularization parameters, together with emerging tools in numerical linear algebra should be dealt in a unified way, in order to allow for a substantial improvement in inversion results. The aim of this minisymposium is to show connections between emerging mathematical research and industrial applications, giving a chance to young researchers to present their results to the Italian industrial mathematics community.

Iterated Tikhonov regularization with operator dependency

Davide Bianchi
Università degli Studi dell'Insubria
via Castelnuovo, 11 22100 - Como Italy
d.bianchi9@uninsubria.it

Marco Donatelli
Università degli Studi dell'Insubria
via Castelnuovo, 11 22100 - Como Italy
marco.donatelli@uninsubria.it

We consider linear operator equations of the form

$$Kx = y\,, \tag{1}$$

where $K : \mathcal{X} \to \mathcal{Y}$ is a compact linear operator between Hilbert spaces $\mathcal{X}$ and $\mathcal{Y}$. We assume y to be attainable, i.e., that problem (1) has a solution $x^\dagger = K^\dagger y$ of minimal norm. Here $K^\dagger$ denotes the (Moore-Penrose) generalized inverse operator of K, which is unbounded when K is compact, with infinite dimensional range. Hence problem (1) is ill-posed and has to be regularized in order to compute a numerical solution. We want to approximate the solution $x^\dagger$ of the equation (1), when only an approximation y^δ of y is available with

$$\|y^\delta - y\| \leq \delta,$$

where δ is called the noise level. Since $K^\dagger y^\delta$ is not a good approximation of $x^\dagger$, we approximate $x^\dagger$ with $x_\alpha^\delta := R_\alpha y^\delta$ where $\{R_\alpha\}$ is a family of continuous operators depending on a parameter α. In that sense, a class of such regularizers are filter based methods that exploit the singular value expansion (s.v.e.) of the operator K, acting on its spectrum in order to diminish the effect of the noise on the reconstructed solution. Indeed, if we indicate with $(\sigma_m; v_m, u_m)_{m\in\mathbb{N}}$ the s.v.e of K, then we can express R_α in the following way

$$R_\alpha y = \sum_{m=1}^{+\infty} f_\alpha(\sigma_m)\sigma_m^{-1}\langle y, u_m\rangle v_m,$$

for every y that belongs to the domain of $K^\dagger$ and where $\{f_\alpha\}_{\alpha\in\mathbb{R}_+}$ is a family of functions (filters) that, under suitable conditions, compensate the exponential decay to zero of the singular values σ_m.
A classical example is the Tikhonov regularization for filter $f_\alpha(\sigma_m) = \frac{\sigma_m^2}{\sigma_m^2+\alpha}$. In the last years new kind of Tikhonov based regularization methods were studied in [2], [4], under the name of Fractional or Weighted Tikhonov, and in [3] in order to dampen the oversmoothing effect on the regularized solution of classic Tikhonov and to exploit the informations carried by the spectrum of the operator. In this talk we will present a generalization for those filters, we will show that the aforementioned methods can be seen as a standard Tikhonov-Phillips filter of the form $f_{\alpha,r}(\sigma_m) = \frac{\sigma_m^2}{\sigma_m^2+\alpha g_r(\sigma_m)}$, with g_r a

function that depends on a new parameter r. We will briefly investigate the regularization and convergence property of the filter and we will study conditions under which the regularization of the embedding operator $j_s : H^s(\Omega) \to L^2(\Omega)$ recover the regularized solution in H^t with $t \leq 2s$, i.e., such that the oversmoothing effect of the Tikhonov filter is reduced and more features of the true solution can be recovered. Through the techniques applied in [1] we introduce the nonstationary variant for this method giving sufficient conditions on the convergence and stability that rely only on the control of the sequences of the parameters α and r. Nonstationary version of Tikhonov methods provides better restorations and let us avoid in some sense the nontrivial problem of finding fine ways to compute the optimal parameter α. Finally, numerical examples will be provided to confirm our theoretical results.

References

[1] D. Bianchi, A. Buccini, M. Donatelli and S. Serra-Capizzano. "Iterated fractional Tikhonov regularization." Inverse Problems 31.5 (2015): 055005.

[2] E. M. Hochstenbach, L. Reichel. "Fractional Tikhonov regularization for linear discrete ill-posed problems." BIT, 51 (1) (2011), 197–215.

[3] T.K. Huckle and M. Sedlacek. "Tikhonov–Phillips regularization with operator dependent seminorms." Numerical Algorithms 60.2 (2012): 339-353.

[4] E. Klann, R. Ramlau. "Regularization by fractional filter methods and data smoothing." Inverse Problems 24 (2) (2008), 025018.

Identifying the magnetic permeability in multi-frequency FDEM data inversion

Patricia Díaz de Alba
Università degli Studi di Cagliari
viale Merello, 92 09123 - Cagliari Italy
patricia.diazdealba@gmail.com

Giuseppe Rodriguez
Università degli Studi di Cagliari
viale Merello, 92 09123 - Cagliari Italy
rodriguez@unica.it

Following some previous papers [1, 2], this work aims to identify, by non destructive investigation of soil properties, inhomogeneities in the ground or the presence of particular conductive substances such as metals, minerals and other geological structures.
One of the most important prospecting techniques in applied geophysics is the one that analyze the propagation of an electromagnetic field into the ground. The *frequency domain electromagnetic* (FDEM) induction analysis utilizes a constant frequency signal and measures the deflection of the EM field produced by eddy currents into the ground. The principle of operation of a ground conductivity meter (GCM) is based on an alternating electrical current which flows through a small electric wire coil (the transmitter). A second coil (the receiver) is positioned at a fixed distance r from the first one, and the two coil axes may be aligned either vertically or horizontally with respect to the ground surface. The transmitting coil generates an electromagnetic field above the surface of the ground, a portion of which propagates into it. This EM field, called the primary field H_P, induces an alternating electrical current within the ground, in turn generating a secondary EM field H_S, which propagates back to the surface and the air above. The second wire coil acts as a receiver, measuring the amplitude and phase components of both the primary and secondary EM fields.
The measurements obtained by a GCM depend on some instrument settings, like the orientation of the dipoles, the frequency of the alternating current, the inter-coil distance, and the height of the instrument above the ground.
We use the following nonlinear model derived from Maxwell's equations, which has been described in [3], to model the interaction of an electromagnetic field with the soil,

$$M_1(\sigma, \mu; h, \omega) = -r^3 \int_0^\infty \lambda^2 e^{-2h\lambda} R_0(\lambda) J_0(r\lambda)\, d\lambda,$$

$$M_2(\sigma, \mu; h, \omega) = -r^2 \int_0^\infty \lambda e^{-2h\lambda} R_0(\lambda) J_1(r\lambda)\, d\lambda.$$

The expression M_1 reproduces the measurements for the coils in the vertical orientation, and M_2 does the same for the horizontal orientation. In the model above, σ and μ are the electrical conductivity and the magnetic permeability of the soil layers, respectively, while h and ω are the height and operating frequency of the device; J_0 and J_1 denote the Bessel functions of the first kind of order 0 and 1, respectively, and R_0 is the reflection

factor, which can be computed by a recursion described in [1].
Starting from electromagnetic induction measurements collected by a GCM, contained in a vector b, we reconstruct the magnetic permeability μ of the soil with respect to depth, extending an algorithm developed in [1] to reconstruct the electrical conductivity σ.
The inverse problem consists of fitting the model to the data, that is determine the permeability vector μ which best approximates the measurements. We minimize with respect to μ the Euclidean norm of the residual between the data and the model, that is,

$$\mu^* = \arg\min_{\mu\in\mathbb{R}^n} \frac{1}{2}\|\mathbf{r}(\mu)\|^2, \qquad \mathbf{r}(\mu) = \mathrm{b} - M_\nu(\mu).$$

where $\nu = 1, 2$ represents the orientation of the device.
The proposed regularized inversion procedure is based on the damped Gauss–Newton method

$$\mu_{k+1} = \mu_k + \alpha_k s_k,$$

where s_k is the solution of the linear squares problem described in [3]

$$\min_{s\in\mathbb{R}^n} \|\mathbf{r}(\mu_k) - J_k s\|,$$

and J_k is the Jacobian matrix. At each step the Jacobian matrix, for which we computed the exact analytical formulae, is approximated via either the truncated value decomposition (TSVD) or the truncated generalized value decomposition (TGSVD).
Various methods are implemented for the automatic estimations of both the truncation parameter k, and the relaxation parameter α_k which ensures the convergence of the method and the positivity of the solution.
Numerical experiments on synthetic data sets illustrate the effectiveness of the method.

References

[1] Deidda, G. P., Fenu, C., and Rodriguez, G. 2014 Regularized solution of a nonlinear problem in electromagnetic sounding. *Inverse Problems.* 30:125014 27 pages.

[2] Díaz de Alba, P. and Rodriguez, G. 2015 Regularized solution of a nonlinear problem in applied Geophysics. In *Proceedings of the XXIV Congress on Differential Equations and Applications / XIV Congress on Applied Mathematics.* ISBN 978–84–9828–527–7. Pages 821–826, Springer.

[3] Díaz de Alba, P. and Rodriguez, G. 2016 Identifying the magnetic permeability in multi-frequency FDEM data inversion. *Work in progress.*

On the computation of the GCV function for Tikhonov Regularization

Caterina Fenu
Università degli Studi di Cagliari
viale Merello, 92 09123 - Cagliari Italy
kate.fenu@unica.it

Lothar Reichel
Kent State University
233 MSB, 1300 Lefton Esplanade, Kent, Ohio 44242
reichel@math.kent.edu

Giuseppe Rodriguez
Università degli Studi di Cagliari
viale Merello, 92 09123 - Cagliari Italy
rodriguez@unica.it

Hassane Sadok
Université du Littoral Côte d'Opale
50 Rue Ferdinand Buisson, 62100 Calais, Francia
Hassane.Sadok@lmpa.univ-littoral.fr

Tikhonov regularization is commonly used for the solution of linear discrete ill-posed problems with error-contaminated data. A regularization parameter, that determines the quality of the computed solution, has to be chosen. One of the most popular approaches to choosing this parameter is to minimize the Generalized Cross Validation (GCV) function. The minimum can be determined quite inexpensively when the matrix A that defines the linear discrete ill-posed problem is small enough to rapidly compute its singular value decomposition (SVD). We are interested in the solution of linear discrete ill-posed problems with a matrix A that is too large to make the computation of its complete SVD feasible. We will present two fairly inexpensive ways to determine upper and lower bounds for the numerator and denominator of the GCV function for large matrices A [1, 2]. The first one is based on Gauss-type quadrature and the second one on a low-rank aproximation of the matrix A. These bounds are used to determine a suitable value of the regularization parameter. Computed examples illustrate the performance of the proposed methods.

References

[1] C. Fenu, L. Reichel, and G. Rodriguez. *GCV for Tikhonov regularization via global Golub-Kahan decomposition*. Numer. Linear Algebra Appl., 23:467-484, 2016.

[2] C. Fenu, L. Reichel, G. Rodriguez and H. Sadok. *GCV for Tikhonov regularization by partial singular value decomposition*. Submitted, 2016.

Regularization matrices via matrix nearness problems

Silvia Noschese
SAPIENZA Università di Roma
Piazzale Aldo Moro, 2 00185 - Roma Italy
noschese@mat.uniroma1.it

Lothar Reichel
Kent State University
Kent OH 44242 - USA
reichel@math.kent.edu

Guangxin Huang
Chengdu University of Technology
Chengdu 610059 - P. R. China
huangx@cdut.edu.cn

This talk is concerned with the solution of large-scale linear discrete ill-posed problems with error-contaminated data. Tikhonov regularization is a popular approach to determine meaningful approximate solutions of such problems. The choice of regularization matrix in Tikhonov regularization may significantly affect the quality of the computed approximate solution. The regularization matrix should be chosen to promote the recovery of known important features of the desired solution, such as smoothness and monotonicity. Common choices of regularization matrices are the identity matrix, and scaled finite difference approximations of the first and second derivative operators. Several approaches to construct regularization matrices with desirable properties are described in the literature; see, e.g., [1, 2, 3, 4, 5]. Many of these approaches are designed to yield square modifications of the above mentioned finite difference matrices that can be applied in conjunction with iterative solution methods based on the Arnoldi process.
We describe a novel approach to determine regularization matrices with desired properties by solving a matrix nearness problem. The constructed regularization matrix is the closest matrix in the Frobenius norm with a prescribed null space to a given square nonsingular matrix.
Numerical examples illustrate the performance of the regularization matrices so obtained.

References

[1] Calvetti, D., Reichel, L. and Shuibi, A. 2005 *Invertible smoothing preconditioners for linear discrete ill-posed problems.* Appl. Numer. Math. 54, 135–149.

[2] Donatelli, M., Neuman, A. and Reichel, L. 2012 *Square regularization matrices for large linear discrete ill-posed problems.* Numer. Linear Algebra Appl. 19, 896–913.

[3] Hansen, P. C. and Jensen, T. K. 2006 *Smoothing norm preconditioning for regularizing minimum residual methods.* SIAM J. Matrix Anal. Appl. 29, 1–14.

[4] Morigi, S., Reichel, L. and Sgallari, F. 2007 *Orthogonal projection regularization operators*. Numer. Algorithms 44, 99–114.

[5] Noschese, S. and Reichel, L. 2012 *Inverse problems for regularization matrices*. Numer. Algorithms 60, 531–544.

Majorization-Minimization for Nonconvex Regularization

Serena Morigi
Università degli Studi di Bologna
P.zza Porta San Donato, 5 40126 - Bologna Italy
serena.morigi@unibo.it

Alessandro Lanza
Università degli Studi di Bologna
P.zza Porta San Donato, 5 40126 - Bologna Italy
alessandro.lanza2@unibo.it

Fiorella Sgallari
Università degli Studi di Bologna
P.zza Porta San Donato, 5 40126 - Bologna Italy
fiorella.sgallari@unibo.it

Ivan Selesnik
Department of Electrical and Computer Engineering, New York University,
Brooklyn, NY 11201, U.S.A.
selesi@nyu.edu

Image restoration belongs to the mathematical class of inverse problems, which is known to be ill-posed, due to either the non-uniqueness of the solution or the numerical instability of the inversion of the blurring operator in case of image restoration. The regularization term alleviates this problem by reflecting some a-priori properties. Many different variational formulations proposed consider a convex regularization term which leads to solutions that can benefit from optimization theory and can be efficiently solved by robust algorithms with guaranteed convergence. On the other hand, it has been shown that non-smooth, non-convex formulations have remarkable advantages over convex regularizations for restoring images, in particular to restore high-quality piecewise constant images with neat edges, at the cost of more challenging numerical solutions [1],[2]. We propose a novel Majorization Minimization (MM) strategy for the solution of a certain class of non-smooth non-convex optimization problems: the objective function is the sum of a strongly convex quadratic (fidelity) term and a non-convex non-smooth regularization term. The class of MM algorithms is based on the principle of successively minimizing upper bounds of the objective function. Each upper bound, or surrogate function, is locally tight at the current estimate, and each minimization step decreases the value of the objective functional. We propose to majorize the non-convex regularizer with a non-convex surrogate function, designed so that the total surrogate function is convex, thus allowing for a tight approximation of the objective function and, hence, for fast convergence and robustness to local minimizers [3],[4]. An efficient algorithm for minimizing the (convex) surrogate function based on Alternating Direction Method of Multipliers will be presented and the analysis of convergence of the proposed CNC-MM proposal is provided. Numerical

experiments show the effectiveness of the proposed method for the solution of nonconvex minimization problems.

References

[1] I. W. Selesnick, A. Parekh, and I. Bayram, Convex 1-D total variation denoising with non-convex regularization, IEEE Signal Proc. Letters, **22(2)** (2015) 141–144.

[2] M. Nikolova, M. K. Ng and C. P. Tam, Fast Non-convex Non-smooth Minimization Methods for Image Restoration and Reconstruction, IEEE Trans. Image Proc., **19(12)** (2010) 3073–3088.

[3] A. Lanza, S. Morigi, F. Sgallari, Convex image denoising via Non-Convex Regularization via parameter selection, Journal of Mathematical Imaging and Vision, 2016, DOI: $10.1007/s10851 - 016 - 0655 - 7$

[4] A. Lanza, S. Morigi, F. Sgallari, Convex image denoising via Non-Convex Regularization, SSVM Proceedings Series: Lecture Notes in Computer Science, Volume 9087, (2015), Eds. Aujol, Jean-François and Nikolova, Mila and Papadakis, Nicolas, DOI $10.1007/978 - 3 - 319 - 18461 - 653$, Springer International Publishing, pp. 666-677.

Microwave imaging in L^p Banach spaces

Emanuele Tavanti
Dip. di Ingegneria Navale, Elettrica, Elettronica e delle Telecomunicazioni, Univ. di Genova
via all'Opera Pia, 11A, 16145 - Genova, Italy
emanuele.tavanti@edu.unige.it

Andrea Randazzo
Dip. di Ingegneria Navale, Elettrica, Elettronica e delle Telecomunicazioni, Univ. di Genova
via all'Opera Pia, 11A, 16145 - Genova, Italy
andrea.randazzo@unige.it

Claudio Estatico
Dipartimento di Matematica, Università di Genova
via Dodecaneso, 35, 16146 - Genova, Italy
estatico@dima.unige.it

Matteo Pastorino
Dip. di Ingegneria Navale, Elettrica, Elettronica e delle Telecomunicazioni, Univ. di Genova
via all'Opera Pia, 11A, 16145 - Genova, Italy
matteo.tastorino@unige.it

Microwave imaging is recently attracting an increasing interest in several application areas [1], such as civil engineering, with special focus on crack detection [2] and georadar systems [3], and biomedical imaging, e.g. for breast cancer [4] diagnosis. However, microwave imaging relies on the solution of an inverse electromagnetic scattering problem, which is notably non-linear and ill-posed [5]. Moreover, when we deal with a numerical implementation, we usually must cope with a high dimensionality deriving from the discretization of the problem, which leads to long computational times [6].
We want to concentrate on quantitative imaging, where the goal is to estimate the dielectric parameter distribution belonging to an unknown scatterer from a set of electric field samples. This kind of algorithm traditionally perform a regularization working inside L^2 Hilbert space, suffering from oversmoothing effects. Therefore, dielectric discontinuities are poorly reconstructed. Recently, a more general approach has been proposed [7], which defines the recovering problem in L^p Banach space leading to the possibility of tuning the p-norm parameter in such a way to favour sharp and sparse solution [8].
In this abstract, the electromagnetic problem is introduced and the proposed inversion procedure is outlined. Several numerical results proving the efficiency of the method will be provided in the talk. The proposed scheme starts from the following pair of Lippmann-Schwinger integral equation [1]:

$$\begin{cases} \underline{E}_{scat}(\underline{r}) = \int_{V_{inv}} \overline{\overline{G}}_b(\underline{r}) \cdot c(\underline{\xi})\, \underline{E}_{tot}(\underline{\xi})\, d\underline{\xi} \quad \underline{r} \in V_{meas} \\ \underline{E}_{inc}(\underline{r}) = \underline{E}_{tot}(\underline{r}) - \int_{V_{inv}} \overline{\overline{G}}_b(\underline{r}, \underline{\xi}) \cdot c(\underline{\xi})\, \underline{E}_{tot}(\underline{\xi})\, d\underline{\xi} \quad \underline{r} \in V_{inv} \end{cases} \tag{1}$$

where V_{inv} is the investigation domain in which the unknown scatterer is placed, V_{meas} is the observation domain where the electric field is sampled, $c = \varepsilon_r - 1$ is the contrast

function (with ε_r is the space-dependent complex relative electric permittivity), $\overline{\overline{G}}_b$ is the dyadic Green tensor for free space, $\underline{E}_{inc}$ is the incident electric field, $\underline{E}_{tot}$ is the total electric field and $\underline{E}_{scat} = \underline{E}_{tot} - \underline{E}_{inc}$ is the scattered electric field. The first equation is known as data equation and it is a first kind Fredholm integral equation, instead the second one is called state equation and it is a second kind Fredholm integral equation. This system is discretized by using the Methods of Moments (MoM) [9], that is V_{inv} is partitioned in N cubic voxels with centers $\{\underline{r}_i^{inv}\}_{i=1}^N$, where the contrast function and the internal electric fields are therein approximated as constant, whereas the external electric fields are picked up in M measurement points $\{\underline{r}_k^{meas}\}_{k=1}^M$ belonging to V_{meas}. Therefore, the following matrix form is obtained:

$$\begin{cases} \underline{E}_{scat}^{ext} = G^{ext} diag_3\left(\underline{c}\right) \underline{E}_{tot}^{int} \\ \underline{E}_{inc}^{int} = \left[I - G^{int} diag_3\left(\underline{c}\right)\right] \underline{E}_{tot}^{int} \end{cases} \tag{2}$$

where $\underline{E}_{scat}^{ext}$, $\underline{E}_{tot}^{int}$, and $\underline{E}_{inc}^{int}$ are arrays collecting the values of the components of the external scattered, internal total and internal incident electric fields on respective sets of points, $\underline{c}$ is a vector containing the contrast function values inside the voxels, G^{ext} and G^{int} are the external and internal Green matrices respectively, and $diag_3\left(\underline{c}\right) = diag_3\left\{\left[\underline{c}^T\ \underline{c}^T\ \underline{c}^T\right]\right\}$. Green matrices elements are the integrals of the Green's dyadic function and can be computed both through numerical integration and analytical approximation [10], taking into account for the singularities arising in $\underline{r} = \underline{\xi}$ [11]. Finally, a non-linear matrix equation, explicitly relating the measured scattered electric field with the unknowns, is obtained as follows:

$$\underline{E}_{scat}^{ext} = G^{ext} diag_3\left(\underline{c}\right) \left[I - G^{int} diag_3\left(\underline{c}\right)\right]^{-1} \underline{E}_{inc}^{int} = F\left(\underline{c}\right) \tag{3}$$

As introduced in [7] the developed inversion strategy is based on an inexact-Newton scheme where the inner solver is a truncated Landweber method in the framework of the L^p Banach spaces, and can be summarized by the following steps (n and l are indexes for Newton and Landweber loops, respectively, and the initial guess is $\underline{c} = \underline{0}$ if no a-priori information is available):

1. Linearize F at $\underline{c}_n$ in order to get the following linear problem:
$$F'_{\underline{c}_n} \underline{h} = \underline{E}_{scat}^{ext} - F\left(\underline{c}_n\right) \tag{4}$$
2. Solve the linear system by using the truncated Landweber method in L^p Banach spaces. The following step (initialized with $\underline{h}_0 = \hat{\underline{h}}_0 = \underline{0}$) is iterated until a proper convergence criterion (e.g., a maximum number of iterations, a threshold on the variation of the estimated unknown $\underline{h}$ or on the respective residuals) is satisfied:
$$\underline{h}_{l+1} = J_q\left[\hat{\underline{h}}_l - \beta F'^{*}_{\underline{c}_n} J_p\left(F'_{\underline{c}_n} \underline{h}_l - \underline{r}_n\right)\right] \tag{5}$$
where $\underline{r}_n = \underline{E}_{scat}^{ext} - F\left(\underline{c}_n\right)$, $F'^{*}_{\underline{c}_n}$ is the adjoint matrix of $F'_{\underline{c}_n}$, $\beta \in \left(0, 2\left\|F'_{\underline{c}_n}\right\|_2^{-2}\right)$ is the relaxation coefficient, $q = p/(p-1)$ is the conjugate of Hölder and J_p, J_q are the normalized duality maps of the L^p and L^q Banach spaces [8], which are explicitly given by:
$$J_x\left(\underline{y}\right) = \begin{cases} \left\|\underline{y}\right\|_x^{2-x} \begin{bmatrix} |y_1|^{x-1} sgn\left(y_1\right) \\ |y_2|^{x-1} sgn\left(y_2\right) \\ \vdots \end{bmatrix} & \underline{y} \neq \underline{0} \\ \underline{0} & \underline{y} = \underline{0} \end{cases} \tag{6}$$

3. Update the solution:

$$\underline{c}_{n+1} = \underline{c}_n + \underline{h} \tag{7}$$

The method terminate when a proper stopping criterion (e.g., a maximum number of iterations, a threshold on the variation of the estimated unknown $\underline{c}$ or on the respective residuals) is met.
The Jacobian matrix $F'_{\underline{c}}$ associated with the operator F can be achieved by Taylor series expansion:

$$\begin{gathered} F\left(\underline{c}+d\underline{c}\right) = G^{ext} diag_3\left(\underline{c}\right)\left[I - G^{int} diag_3\left(\underline{c}\right)\right]^{-1} \underline{E}^{int}_{inc} + \\ + \underbrace{G^{ext}\left[I - diag_3\left(\underline{c}\right) G^{int}\right]^{-1} diag_3\left(d\underline{c}\right)\left[I - G^{int} diag_3\left(\underline{c}\right)\right]^{-1} \underline{E}^{int}_{inc}}_{F'_{\underline{c}} d\underline{c}} + O\left[diag_3\left(d\underline{c}^2\right) \underline{E}^{int}_{inc}\right] \end{gathered} \tag{8}$$

It follows that:

$$F'_{\underline{c}} = G^{ext}\left[I - diag_3\left(\underline{c}\right) G^{int}\right]^{-1} diag_3\left\{\left[I - G^{int} diag_3\left(\underline{c}\right)\right]^{-1} \underline{E}^{int}_{inc}\right\} \tag{9}$$

In our talk, we will show the application of the proposed approach on simple dielectric configurations to the aim of highlighting algorithm's performances both in terms of accuracy, with particular reference to the traditional regularization in L^2 Hilbert space, and computational times, where this last critical issue will lead to the introduction of proper speeding up techniques.

References

[1] Pastorino, M. 2010 *Microwave imaging.* Hoboken, N.J.: Wiley.

[2] Randazzo, A and Estatico, C. 2012 *A regularisation scheme for electromagnetic inverse problems: application to crack detection in civil structures.* Nondestructive Testing and Evaluation, vol. 27, no. 3, pp. 189–197.

[3] Estatico, C. et al. 2015 *A Multifrequency Inexact-Newton Method in L^p Banach Spaces for Buried Objects Detection.* IEEE Transactions on Antennas and Propagation, vol. 63, no. 9, pp. 4198–4204.

[4] O'Halloran, M. et al. 2010 *Quasi-Multistatic MIST Beamforming for the Early Detection of Breast Cancer.* IEEE Transactions on Biomedical Engineering, vol. 57, no. 4, pp. 830–840.

[5] Bertero, M. and Boccacci, P. 1998 *Introduction to inverse problems in imaging.* Bristol, UK: IOP Publishing.

[6] Tavanti, E. et al. 2015 Nonlinear electromagnetic inverse scattering in Lp via Frozen or Broyden update of the Frechet derivative. In *Proceedings of the "NCMIP 2015: 5th International Workshop on New Computational Methods for Inverse Problems"* , J. of Phys.: Conf. Series, 657, IOP (2015) 012008.

[7] Estatico, C. et al. 2012 *A novel microwave imaging approach based on regularization in Lp Banach spaces.* IEEE Transactions on Antennas and Propagation, vol. 60, no. 7, pp. 3373–3381.

[8] Schuster, T. 2012 *Regularization methods in Banach spaces.* Berlin: De Gruyter.

[9] Harrington, R. F. 1993 *Field Computation by Moment Methods.* Piscataway, NJ: Ieee.

[10] Livesay, D. E. and Chen, K. 1974 *Electromagnetic Fields Induced Inside Arbitrarily Shaped Biological Bodies.* IEEE Transactions on Microwave Theory and Techniques, vol. 22, no. 12, pp. 1273–1280.

[11] Van Bladel, J. 1961 *Some remarks on green's dyadic for infinite space.* IRE Transactions on Antennas and Propagation, vol. 9, no. 6, pp. 563–566.

Geophysical Multiphase Flows - Part I

PROPOSERS

Augusto Neri
Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Pisa
Via della Faggiola 32, 56126 Pisa, Italy
augusto.neri@ingv.it

Enrique D. Fernández-Nieto
Dpto. Matemática Aplicada I, Universidad de Sevilla
Avda. Reina Mercedes N.2, Sevilla, Spain
edofer@us.es

SPEAKERS

Lorenzo Valdettaro (keynote)
Dip. di Matematica, Politecnico di Milano
lorenzo.valdettaro@polimi.it

Matteo Cerminara
Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Pisa
matteo.cerminara@ingv.it

Gladys Narbona-Reina
Dpto. Matemática Aplicada I, Universidad de Sevilla
gnarbona@us.es

Augusto Neri
Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Pisa
augusto.neri@ingv.it

Paul Vigneaux
E.N.S. Lyon
paul.vigneaux@math.cnrs.fr

Many geological and geophysical events are characterized by a strongly non-homogeneous nature of the medium. Some of these include volcanic processes, such as plumes, pyroclastic density currents and lava flows, debris flows and sediment transport, submarine avalanches, ice formation among others. In order to properly describe their dynamics and hazards multiphase flow models are needed. Such models allow to describe mechanical and thermal non-equilibrium effects between the different phases of the mixture as well as represent complex inter-phase processes such as particle drag, aggregation and sedimentation. In this minisymposium, recent advances on the modelling and numerical simulation of geophysical multiphase flows will be illustrated together with some application to the above described processes.

A multiphase model suitable for the numerical simulation of ice production in turbulent water

Lorenzo Valdettaro
MOX-Modelling and Scientific Computing, Dipartimento di Matematica, Politecnico di Milano
Via Bonardi 9, 20133, Milano, Italy
lorenzo.valdettaro@polimi.it

Antonella Abbà
Dipartimento di Scienze e Tecnologie Aerospaziali, Politecnico di Milano
Via La Masa 34, 20156, Milano, Italy
antonella.abba@polimi.it

Luca Bonaventura
MOX-Modelling and Scientific Computing, Dipartimento di Matematica, Politecnico di Milano
Via Bonardi 9, 20133, Milano, Italy
luca.bonaventura@polimi.it

Vanessa Covello
Dipartimento di Scienze e Tecnologie Aerospaziali, Politecnico di Milano
Via La Masa 34, 20156, Milano, Italy
vanessa.covello@polimi.it

Alessandro Della Rocca
MOX-Modelling and Scientific Computing, Dipartimento di Matematica, Politecnico di Milano
Via Bonardi 9, 20133, Milano, Italy.
Tenova S.p.A., Via Albareto 31, 16135, Genova, Italy.
alessandro.dellarocca@polimi.it
alessandro.dellarocca@tenova.com

Ice formation in the ocean and sea is a complex phenomenon, whose correct description is essential in order to model adequately the atmosphere-ocean heat fluxes, the salt rejection phenomena and the damping and mixing effects due to turbulent convection. Moreover, ice formation greatly affects the geophysical and biological processes occurring in the polar oceans, and could produce serious damages to hydroelectric facilities in rivers. In this talk we present a multiphase model able to describe all the stages of ice production, allowing us to obtain a more realistic prediction of the ice formation process, overcoming the limitation of previous attempts, see e.g.[6, 7, 10, 11], mainly based on the Boussinesq approximation (which implies low ice concentration). The proposed model considers the mixture of ice and water as a two-phase dense compressible fluid. The behaviour of water is modelled by means of an equation of state that links its density to temperature, salinity and pressure, using a reduced form derived from Brydon et al. [3], our reduced equation is valid in a limited pressure range, which however corresponds to water depths of the order of hundreds of meters, therefore in the range of interest for our study. In particular,

in [3] the following form of the equation of state is proposed,

$$\begin{aligned}\rho(\theta,S,p) =& \rho_0 + C_1(p) + C_2(p)\,\theta + C_3(p)\,S + C_4(p)\,\theta^2 \\ &+ C_5(p)\,S\theta + C_6(p)\,\theta^3 + C_7(p)\,S\theta^2,\end{aligned} \tag{1}$$

where θ is the potential temperature, whereas $C_n(p) = a_n + b_n p + c_n p^2$, with coefficients given in [3]. This equation has been found to be valid for $-2°C < \theta < 40°C$, 0 psu$< S <$ 42 psu. Our equation is linearized with respect to p:

$$\rho_r(T,S,p) = (b_5 TS + b_2 T + b_1)\,p + a_5 TS + a_4 T^2 + a_3 S + a_2 T + a_1 + \rho_0, \tag{2}$$

where $\rho_0 = 1000\ kg/m^3$ denotes the reference density. Figure 1 compares the behaviour of the reduced form of the equation of state, with the original one Eq.(1). The comparison has been carried out in term of density anomaly $(\rho - \rho_0)$, at $p = 100$ decibars (depth about 100 meters), for different values of salinity ($S = 0, 25, 40$ psu).

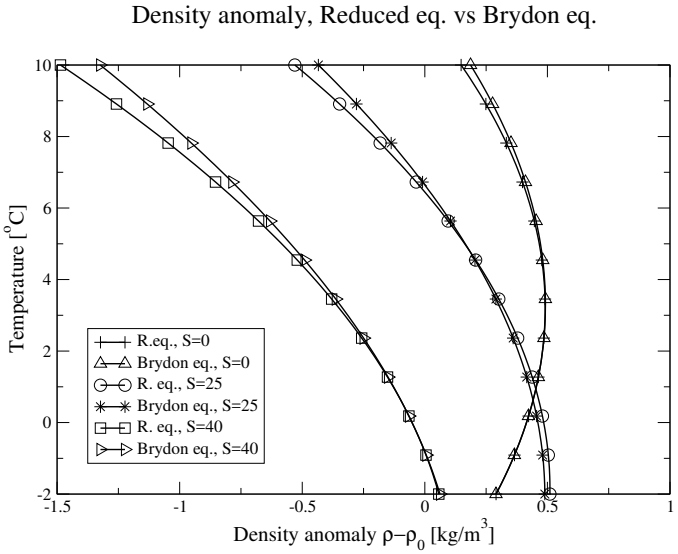


Figure 1: Behaviour of the reduced form Eq.(2) and the original form Eq.(1) in the $((\rho - \rho_0), T)$ plane for $S = 0, 25, 40$ psu, at $p = 100$ decibars.

Our multiphase model wants to reproduce the interaction phenomena occurring between phases when the ice volume fraction is large, including in the momentum equations additional terms, related to the drag force between liquid and particles, and to the particle-particle interaction force. For this purpose, we use a sophisticated modelling approach, typically adopted for the numerical simulation of liquid-solid multiphase flows of industrial interest, see e.g.[4, 9, 8]. The model equations read

$$\frac{\partial}{\partial t}\Big[(1-\phi_I)\,\rho_W\Big] + \frac{\partial}{\partial x_i}\Big[(1-\phi_I)\,\rho_W u_i\Big] = S_{mass}, \tag{3}$$

$$\frac{\partial}{\partial t}(\phi_I \rho_I) + \frac{\partial}{\partial x_i}(\phi_I \rho_I v_i) = -S_{mass}. \tag{4}$$

$$\begin{aligned}\frac{\partial}{\partial t}\Big[(1-\phi_I)\,\rho_W u_i\Big] + \frac{\partial}{\partial x_j}\Big[(1-\phi_I)\,\rho_W u_j u_i\Big] + f^{cor}_{i,j} u_j = &-(1-\phi_I)\frac{\partial \bar{p}}{\partial x_i} + (1-\phi_I)\frac{\partial \tau_{ij}}{\partial x_j} \\ &+ F_i^W + (1-\phi_I)\,\bar{\rho}_W g_i + S_{mom},\end{aligned} \tag{5}$$

$$\frac{\partial}{\partial t}\left(\phi_I \rho_I v_i\right) + \frac{\partial}{\partial x_j}\left(\phi_I \rho_I v_j v_i\right) + f_{i,j}^{cor} v_j = -\phi_I \frac{\partial \bar{p}}{\partial x_i} + \phi_I \frac{\partial \tau_{ij}}{\partial x_j} + F_i^I + \phi_I \rho_I g_i - S_{mom}, \quad (6)$$

$$\frac{3}{2}\left[\frac{\partial}{\partial t}\left(\rho_I \phi_I \Theta\right) + \frac{\partial}{\partial x_i}\left(\rho_I \phi_I v_i \Theta\right)\right] = \left[-p_s \delta_{ij} + \tau_{s,ij}\right] \frac{\partial v_i}{\partial x_j} - \frac{\partial}{\partial x_i}\left(k_\Theta \frac{\partial \Theta}{\partial x_i}\right) - \Gamma_\Theta. \quad (7)$$

$$\frac{\partial}{\partial t}\Big[\left(1-\phi_I\right) T_W\Big] + \frac{\partial}{\partial x_i}\Big[\left(1-\phi_I\right) u_i T_W\Big] = \frac{\partial}{\partial x_i}\left(\left(1-\phi_I\right) k_t \frac{\partial T_W}{\partial x_i}\right) + \phi_I \lambda_t \left(T_I - T_W\right) + S_T. \quad (8)$$

$$\frac{\partial}{\partial t}\Big[\left(1-\phi_I\right) S\Big] + \frac{\partial}{\partial x_i}\Big[\left(1-\phi_I\right) S u_i\Big] = \frac{\partial}{\partial x_i}\left(\left(1-\phi_I\right) k_s \frac{\partial S}{\partial x_i}\right) + S_{sal}, \quad (9)$$

Where Eqs. (3) and (5) denote the mass and momentum conservation for water, and Eqs. (4) and (6) are the corresponding equations for ice. Eq.(7) describes the evolution of granular temperature for ice $\Theta = \frac{1}{3}\langle C^2 \rangle$, where C is the deviation of the ice particles velocity from their mean velocity and the operator $\langle\ \rangle$ denotes the mean value based on the Gaussian distribution. The set of equations is completed by the evolution equation for the water temperature Eq.(8) and for salinity Eq.(9). The subscripts $_W$ and $_I$ denote respectively water and ice; u_i and v_i are the water and ice velocities, ϕ_I is the ice volume fraction and $\bar{p}$ is the pressure deviation from the hydrostatic one. S_{mass}, S_{mom}, $S_T + \phi_I \lambda_t \left(T_I - T_W\right)$, Γ_θ, S_{sal} denote the source terms that account for the phase transition and the interaction phenomena between ice particles. Finally, F_i^W and F_i^I stand for the drag and interaction terms among the species.
In order to obtain an accurate prediction of ice production in turbulent water convection, the multiphase model is coupled with the Large Eddy Simulation (LES) technique.

In view of the numerical discretization, a low-Mach number asymptotic analysis has been performed. The divergence constraint condition for the velocity field of continuous phase has been imposed on the zero-Mach number equations by means of a projection method for incompressible variable density flows, derived from [5, 2]. The governing equations are discretized using the finite volume method, by the OpenFOAM tool. As a starting point toward the development of the multiphase numerical solver, we develop a finite volume solver, to be valid in the Boussinesq limit (which implies low ice concentration). The predictive capabilities of this solver have been verified by means of a comparison with numerical solutions obtained on the Rayleigh-Bénard convection problem by a finite difference numerical code [1]. Preliminary results in the non-Boussinesq regime (large ice concentration) will also be presented.

References

[1] Abbà, A. Olla, P. and Valdettaro, L. 2014 *Numerical Analysis of Frazil Ice Formation in Turbulent Convection.* Progress in Turbulence VI, Proceedings of the iTi Conference on Turbulence, Springer Proceedings in Physics, 165.

[2] Bell, J.B. and Marcus, D.L. 1992 *A second-order projection method for variable-density flows.* J. Comput. Phys., 101, pp. 334–348.

[3] Brydon, D. Sun, S. and Bleck, R. 1999 *A new approximation of the equation of state for seawater, suitable for numerical ocean models.* JGR-Oceans (1978-2012), 104.C1, 1537–1540.

[4] Gidaspow, D. 1994 *Multiphase Flow and Fluidization*. Academic Press, San Diego.

[5] Ham, F. and Iaccarino, G. 2004 *Energy conservation in colocated discretization schemes on unstructured meshes*. Ann. Rev. Brief 2004, CTR, NASA, Ames/Stanford University.

[6] Holland, P.R. and Feltham, D.L. 2005 *Frazil dynamics and precipitation in a water column with depth-dependent supercooling*. J. Fluid Mech. 530, 101–124.

[7] Jenkins, A. and Bombosch, A. 1995 *Modeling the effects of frazil ice crystals on the dynamics and thermodynamics of ice shelf water plumes*. JGR-Oceans (1978-2012). 100.C4, 6967–6981.

[8] Jenkins, J.J. and Savage, S.B. 1983 *A theory for the rapid flow of identical smooth nearly elastic spherical particles*. J. Fluid Mech. 130, 187–202.

[9] Lun, C.K.K. Savage, S.B. and Chepurning N., 1984 *Kinetic theories for granular flow: Inelastic particles in Couette flow and singly inelastic particles in a general flow field*. J. Fluid Mech. 140, 223–256.

[10] Omstedt, A. and Svensson, U. 1984, *Modeling supercooling and ice formation in a turbulent Ekman layer*. JGR-Oceans (1978-2012). 89.C1, 735–744.

[11] Skyllingstad, E.D. and Denbo, D.W. 2001 *Turbulence beneath sea ice and leads: A coupled sea ice/Large-Eddy Simulation study*. JGR-Oceans (1978–2012). 106.C2, 2477–2497.

Large eddy simulation of gas-particle kinematic decoupling in volcanic plumes and pyroclastic density currents by using the equilibrium-Eulerian approach

Matteo Cerminara
Istituto Nazionale di Oceanografia e Geofisica Sperimentale
Istituto Nazionale di Geofisica e Vulcanologia
via della Faggiola, 32 56126 - Pisa, Italy
mcerminara@inogs.it

Tomaso Esposti Ongaro
Istituto Nazionale di Geofisica e Vulcanologia
via della Faggiola, 32 56126 - Pisa, Italy
tomaso.espostiongaro@ingv.it

Augusto Neri
Istituto Nazionale di Geofisica e Vulcanologia
via della Faggiola, 32 56126 - Pisa, Italy
augusto.neri@ingv.it

We present three-dimensional (3D) numerical simulations of turbulent gas–particle flows generated during explosive eruptions. They are carried out with the ASHEE (ASH Equilibrium Eulerian) model, a CFD solver we implemented in the OpenFOAM infrastructure [1]. The ASHEE model solves the compressible balance equations of mass, momentum, and enthalpy of a gas-particle mixture and it is able to describe the kinetic decoupling for particles characterized by Stokes number (i.e., the ratio between the particle equilibrium time and the flow characteristic time) below about 0.2 (or particles smaller than about 1 mm). The computational fluid dynamic model is designed to accurately simulate a turbulent flow field by using a Large Eddy Simulation approach, and it is thus suited to analyze the role of particle non-equilibrium in the dynamics of turbulent volcanic plumes [2] and dilute pyroclastic density currents.

Two end member scenarios for volcanic plumes are analyzed, with mass eruption rate equal to $1.5 * 10^6$ kg/s (weak plume) and $1.5 * 10^9$ kg/s (strong plume) in the absence of wind [3, 4]. For each scenario, we compare the 3D results, averaged in space and time, with theoretical results obtained from integral plume models [5]. Such an approach allows to refine empirical parameters used by simplified integral models. Moreover, we quantitatively evaluate the effects of gas-particle non-equilibrium processes on the large-scale plume dynamics and the related computational errors. We show that particle kinematic gas–particle non-equilibrium introduces a novel phenomenon, that we have called *jet-dragging*, associated with the bulk inertial deceleration of the mixture in the volcanic jet region [2]. Coarse ash particles drag the other phases upwards, shifting up plume mean profiles by about 20-25% in the present application. Preferential concentration (i.e. the normalized ratio between the local particle concentration and the concentration of a tracer) ranges between 0.05 and 5 for 1 mm particles, i.e., density fluctuates by up to two orders of magnitude due to particle clustering.

The same approach has been applied to gravity currents [6] and dilute pyroclastic density currents, by adding a boundary condition for the sedimentation of ash particles, in order to avoid the formation of a basal concentrated layer where the equilibrium–Eulerian approximation is no longer valid.

This approach allows to quantify non-equilibrium effects in polydispersed volcanic mixtures without the need of solving the full Eulerian–Eulerian [7] equations.

References

[1] Cerminara, M., Esposti Ongaro, T. and Berselli, L. C. 2016. *ASHEE-1.0: a compressible, equilibrium–Eulerian model for volcanic ash plumes.* Geosci. Model Dev. 9, 697–730.

[2] Cerminara, M., Esposti Ongaro, T. and Neri, A. 2016. *Large eddy simulation of gas-particle kinematic decoupling and turbulent entrainment in volcanic plumes.* J. Volcanol. Geotherm. Res, accepted.

[3] Costa, A. et al. 2016. *Results of the eruptive column model inter-comparison study.* J. Volcanol. Geotherm. Res., in press.

[4] Suzuki, Y. J. et al. 2016. *Inter-comparison of three-dimensional models of volcanic plumes.* J. Volcanol. Geotherm. Res., accepted.

[5] Cerminara, M. 2015. *The Multiphase Buoyant Plume Solution of the Dusty Gas Model.* ArXiv:1506.01638.

[6] Berselli, L. C., Cerminara, M. and Iliescu, T. 2015. *Disperse Two-Phase Flows, with Applications to Geophysical Problems.* Pure Appl. Geophys. 172, 181–196.

[7] Esposti Ongaro, T. and Cerminara, M. 2016. *Non-equilibrium processes in ash-laden volcanic plumes: new insights from 3D multiphase flow simulations.* J. Volcanol. Geotherm. Res., in press.

A two-phase three-layers depth-averaged model with mass exchange for sediment transport problems

Gladys Narbona-Reina
Dpto. Matemática Aplicada I. Universidad de Sevilla
Avda. Reina Mercedes 2, 41012 - Sevilla Spain
gnarbona@us.es

Luca Bonaventura
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
Luca.Bonaventura@polimi.it

Enrique D. Fernández-Nieto
Dpto. Matemática Aplicada I. Universidad de Sevilla
Avda. Reina Mercedes 2, 41012 - Sevilla Spain
edofer@us.es

The objective of this work is to deduce a mathematical model for the sediment transport in rivers. Most of the models in the literature concerning this issue hold some of the different kind of transport occurred in rivers: bed-load, suspended-load or wash-load. Additionally, some of them treat the task of the mass exchange in this system what becomes one of the more important effect to be considered.

The whole physical system includes particles moving as bed load, suspended load and wash load, which is seen indeed as a subset of the suspended load. In the literature on this topic, several proposals to tackle the modelling of the sediment transport have been advanced. In general, the basis are the two-layer and two-phase models. The two-layer models are based on the fact that the different sediment transport types can be seen as separate layers with some kind of interactions among them. The two-phase models keep the property of one fluid formed up of two different components that interacts intrinsically, water and sediment, so the total column is seen as a mixture. Of course, both kind of models are not incompatible and the suitability of each one depends on the physical situations that one would like to focus on.

Furthermore, in this type of geophysical problems, the derivation of depth-integrated models −under the assumption of shallow flows− are extendedly accepted in order to get models mathematically and numerically manageable together with a good review in results that captures the essential effects.

In this work we propose a complete model that describes the three phenomena, washed, suspended and bed load sediment transport, as well as the interactions between them. For this aim we use several mathematical tools in order to take into account the physical environment of the problem: depth-average, asymptotic approximation, different time scales for hydrodynamic and morphodynamic components, mass and momentum conservation.

We consider the fluid-solid mixture model proposed by Jackson [5] as a basis and we follow different derivations to obtain the dynamics for the three layers. The top layer is

defined as a wash layer with small particle concentrations, so we derive a two-phase model based on [3, 2] considering same velocity for both phases. For the middle suspension layer, made up of water and grains, we also obtain a two-phase model but in this case we keep the different velocity for each phase. For the layer below, we follow the derivation developed in [1] to obtain an Exner type model for arbitrary sloping beds.
Erosion, suspension and deposition are considered in the whole system through appropriate boundary conditions. In order to well define the exchange of mass between sediment layers, mass and momentum conservation at the interface are imposed. The rate of erosion/deposition/suspension are defined following [6, 4]. Thus, this model can be seen as a generalization of the existing models. Finally, several numerical tests will be presented.

References

[1] Fernández-Nieto, E.D.; Morales de Luna, T.; Narbona-Reina, G. and Zabsonré, J.D. 2016 *Formal deduction of the Saint-Venant-Exner model in- cluding arbitrarily sloping sediment beds and associated energy.* Accepted in ESAIM: M2AN, doi:10.1051/m2an/2016018.

[2] Garegnani, G.; Rosatti, G. and Bonaventura, L. 2011 *Free surface flows over mobile bed: mathematical analysis and numerical modeling of coupled and decoupled approaches.* Communications In Applied And Industrial Mathematics, 2(1).

[3] Garegnani, G.; Rosatti, G. and Bonaventura, L. 2013 *On the range of validity of the Exner-based models for mobile-bed river flow simulations.* Journal of Hydraulic Research, 51:4, 380−391.

[4] Iverson, R. M., and Ouyang, C. 2015 *Entrainment of bed material by Earth-surface mass flows: Review and reformulation of depth-integrated theory.* Rev. Geophys., 53, 27−58, doi:10.1002/2013RG000447.

[5] Jackson, R. 2000 *The Dynamics of Fluidized Particles.* Cambridge University Press, Cambridge.

[6] Zech, Y.; Soares-Frazão, S.; Spinewine, B.; Savary, C. and Goutire, L. 2009 *Inertia effects in bed-load transport models.* Can.J.Civ.Eng. 36, 1587−1597.

Modelling polydispersity and aggregation processes through the method of moments: application to volcanic plumes

Augusto Neri
Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Pisa
via della Faggiola, 32 56126 - Pisa Italy
augusto.neri@ingv.it

Mattia de' Michieli Vitturi
Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Pisa
via della Faggiola, 32 56126 - Pisa Italy
mattia.demichielivitturi@ingv.it

Numerical modelling of volcanic processes has greatly advanced in the last decades and models are now often able to deal with the multiphase nature of the eruptive mixture. Nevertheless, the wide polidispersity of multiphase mixtures is often ignored or oversimplified. In volcanic plume dynamics, for example, the grain-size distribution of pyroclasts is generally neglected (i.e. the mixture is approximated as a pseudo-gas) or simplified by a discretization in a limited number of classes (phases). Such an approach do not allow to describe the continuous variability of fundamental physical and chemical properties of the dispersed phases (typically solid or liquid particles) or the aggregation and fragmentation processes that commonly occur within volcanic plumes.
In this talk we present a theoretical framework, and corresponding computational models, namely the method of moments, to fully describe the continuous nature of volcanic multiphase mixtures [2, 3]. The method allows to track the evolution of the particles size distribution through a population balance equation. Such equation is formulated in terms of a density function and then some integral quantities of interest (i.e. the moments) are derived and their transport equations are formulated.
The model presented describes an extension of the simple plume theory [4] to the steady-state 1D dynamics of volcanic plumes based on the method of moments [1]. Aggregation is introduced in the population balance equation following the approach of [5]. The aggregation functions and kernels are based on simplified theoretical models and laboratory experiments describing the behavior of ash particles transported in turbulent gaseous flow.
The effects of source conditions at the volcanic vent and particle aggregation, in terms of variation of the parameters of the grain-size distribution along the plume, will be illustrated and discussed with the aim to present the main outcomes as well as the potentiality and limitations of the approach.

References

[1] de' Michieli Vitturi, M., Neri, A. and Barsotti, S. 2015 *PLUME-MoM 1.0: A new integral model of volcanic plumes based on the method of moments*. Geosci. Model Dev., Copernicus GmbH, 8, 2447?2463.

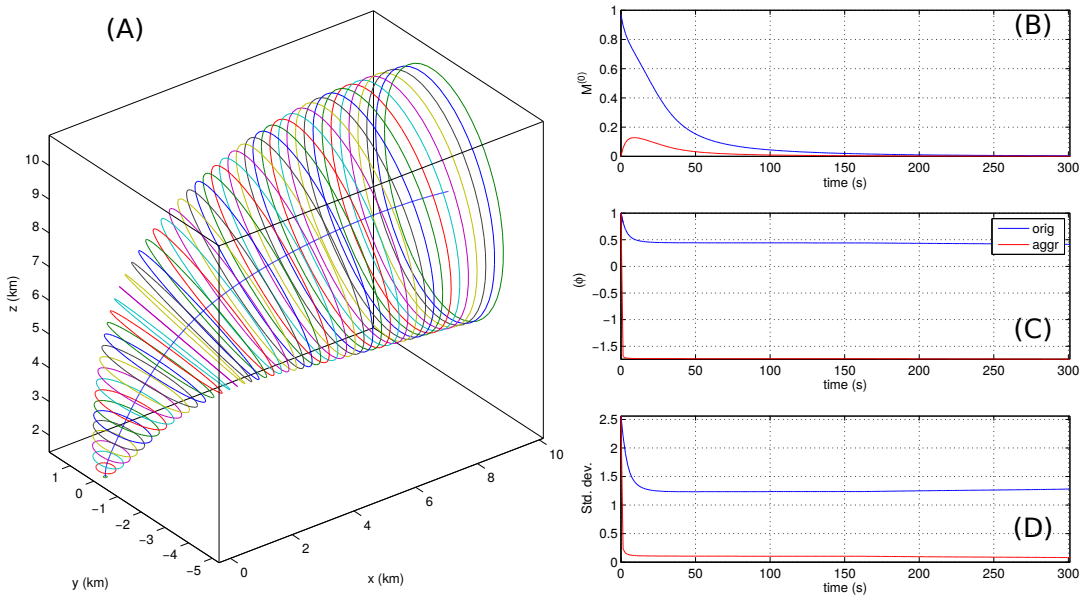


Figure 1: Results of the PlumeMoM for a weak plume. (A) Cross-sectional areas; (B) number of non-aggregated (blue line) and aggregated (red line) particles vs ascent time; (C) mean size in the Krumberin scale of non-aggregated (blue line) and aggregated (red line) particles vs ascent time; (C) standard deviation of the size in the Krumberin scale of non-aggregated (blue line) and aggregated (red line) particles vs ascent time.

[2] Hulburt, H. M. and Katz, S. 1964 *Some problems in particle technology: A statistical mechanical formulation.* Chemical Engineering Science, Elsevier, 19, 555–574.

[3] Marchisio, D. L. and Fox, R. O. 2013 *Computational Models for Polydisperse Particulate and Multiphase Systems.* Cambridge University Press.

[4] Morton, B. 1959 *Forced plumes.* Journal of Fluid Mechanics, Cambridge Univ Press, 5, 151–163.

[5] Smoluchowski, M. v. 1917 *Grundriß der Koagulationskinetik kolloider Lösungen.* Colloid & Polymer Science, 21-3, 98–104.

Numerical schemes of viscoplastic avalanches. A shallow - Bingham flow model.

Paul Vigneaux
Ecole Normale Superieure de Lyon
46 allee d'Italie, 69364 - Lyon France
Paul.Vigneaux@math.cnrs.fr

Enrique D. Fernández-Nieto
Universidad de Sevilla, Spain
edofer@us.es

Jose Maria Gallardo
Universidad de Malaga, Spain
jmgallardo@uma.es

In this talk, we describe the numerical resolution of a shallow water viscoplastic flow model. Viscoplastic materials are characterized by the existence of a yield stress: below a certain critical threshold in the imposed stress, there is no deformation and the material behaves like a rigid solid, but when that yield value is exceeded, the material flows like a fluid. In the context of avalanches, it means that after going down a slope, the material can stop and its free surface has a non-trivial shape, as opposed to the case of water (Newtonian fluid). The model involves variational inequalities associated with the yield threshold: finite-volume schemes are used together with duality methods (namely Augmented Lagrangian and Bermudez-Moreno) to discretize the problem. To be able to accurately simulate the stopping behaviour of the avalanche, new schemes need to be designed, involving the classical notion of well-balancing. In the present context, it needs to be extended to take into account the viscoplastic nature of the material as well as general bottoms with wet/dry fronts which are encountered in geophysical geometries. [1]

References

[1] Enrique D. Fernandez-Nieto, Jose M. Gallardo, Paul Vigneaux. *Efficient numerical schemes for viscoplastic avalanches. Part 1: the 1D case.* Journal of Computational Physics, 2014, Vol. 264, pp 55-90.

Geophysical Multiphase Flows - Part II

PROPOSERS

Augusto Neri
Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Pisa
Via della Faggiola 32, 56126 Pisa, Italy
augusto.neri@ingv.it

Enrique D. Fernández-Nieto
Dpto. Matemática Aplicada I, Universidad de Sevilla
Avda. Reina Mercedes N.2, Sevilla, Spain
edofer@us.es

SPEAKERS

Caterina Bassi
Politecnico di Milano
caterina.bassi@polimi.it

Léa Boittin
INRIA Paris
lea.boittin@student.ecp.fr

Vito Zago
Istituto Nazionale di Geofisica e Vulcanologia
vito.zago@ingv.it

Cipriano Escalante
Dpto. Análisis Matemático, Universidad de Málaga
escalante@uma.es

Enrique D. Fernández-Nieto
Dpto. Matemática Aplicada I, Universidad de Sevilla
edofer@us.es

Piero Olla
ISAC-CNR, Cagliari
olla.dsf@unica.it

Many geological and geophysical events are characterized by a strongly non-homogeneous nature of the medium. Some of these include volcanic processes, such as plumes, pyroclastic density currents and lava flows, debris flows and sediment transport, submarine avalanches, ice formation among others. In order to properly describe their dynamics and hazards multiphase flow models are needed. Such models allow to describe mechanical and thermal non-equilibrium effects between the different phases of the mixture as well as represent complex inter-phase processes such as particle drag, aggregation and sedimentation. In this minisymposium, recent advances on the modelling and numerical simulation of geophysical multiphase flows will be illustrated together with some application to the above described processes.

Dynamic Models for Large Eddy Simulation of variable density compressible flows with a high order DG method

Caterina Bassi
MOX - Modelling and Scientific Computing, Dipartimento di Matematica, Politecnico di Milano
via Bonardi, 9 20133 - Milano Italy
caterina.bassi@polimi.it

Antonella Abbà
Dipartimento di Scienze e Tecnologie Aerospaziali, Politecnico di Milano
via La Masa, 34 20156 - Milano Italy
antonella.abba@polimi.it

Luca Bonaventura
MOX - Modelling and Scientific Computing, Dipartimento di Matematica, Politecnico di Milano
via Bonardi, 9 20133 - Milano Italy
luca.bonaventura@polimi.it

Marco Restelli
NMPP - Numerische Methoden in der Plasmaphysic, Max-Planck-Institut für Plasmaphysic
Boltzmannstraße, 2 D-85748 - Garching Germany
marco.restelli@ipp.mpg.de

Lorenzo Valdettaro
MOX - Modelling and Scientific Computing, Dipartimento di Matematica, Politecnico di Milano
via Bonardi, 9 20133 - Milano Italy
lorenzo.valdettaro@polimi.it

The impact of dynamic models for applications to LES of compressible variable density flows is assessed in the framework of a numerical model based on high order discontinuous finite elements.
High order finite element methods appear as extremely appealing to implement LES models of turbulent flows due to their potential for reducing the impact of numerical dissipation on most of the spatial scales of interest. Moreover they provide a natural framework to generalise LES filters to arbitrary computational meshes. Following the Variational Multiscale (VMS) approach [7], the filter operation, that is the key tool in LES, can be indeed identified with the projection operator on a finite dimensional space related to the discretization.
We consider the results presented in [1] as a starting point: in this recent work different dynamic models (standard isotropic models [4], anisotropic dynamic model [2]) are tested in a DG-VMS approach for channel flows. In the present investigation the same code and LES models are employed for the simulation of variable density compressible flows and in particular for the simulation of gravity-current fronts in the lock-exchange configuration. In the lock-exchage test case the rectangular domain is initially divided into two regions:

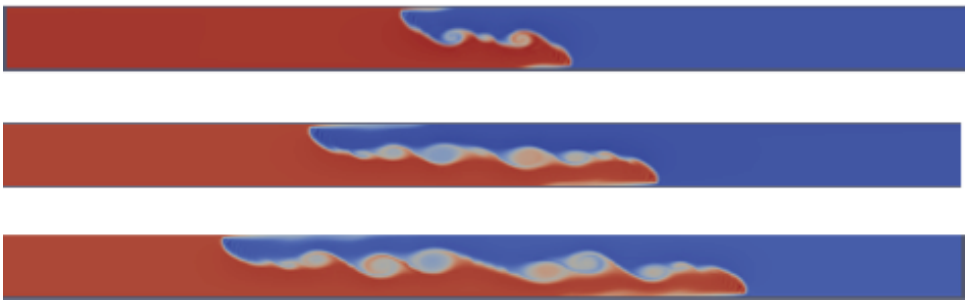


Figure 1: Density profiles obtained at time $t = 5$ (top), $t = 10$ (middle), $t = 15$ (bottom).

the left-hand region is filled with with a fluid characterized by greater density, while the right-hand region contains fluid of smaller density.
The fluid motion is characterized by a dense current that moves rightward along the lower boundary, while the light fluid propagates leftward along the upper boundary. As an example in figure 1 the density profiles obtained at $t = 5$, 10, 15 for a ratio between densities equal to $\gamma = 0.96$ (which satisfies the Boussinesq approximation) are shown.
The results obtained with the compressible DG code are compared with the results obtained in the incompressible regime both for the Boussinesq approximation [6] [8] and for non-Boussinesq flows [3]. As regard as future developments the lock-exchange test case will be employed to test the new compressible eddy viscosity formulation proposed in [5].

References

[1] Abbá A., Bonaventura L., Nini M. and Restelli M. 2015 *Dynamic Models for Large Eddy Simulation of compressible flows with a high order DG method*. Computers and Fluids 122, 209–222.

[2] Abbá A., Cercignani C. and Valdettaro L. 2003 *Analysis of Subgrid Scale Models*. Computer and Mathematics with Applications 46, 521–535.

[3] Birman V.K., Martin J.E. and Meiburg E. 2005 *The non-Boussinesq lock-exchange problem. Part 2. High resolution simulations*. Journal of Fluid Mechanics 537, 125–144.

[4] Germano M., Piomelli U., Moin P. and Cabot W.H. 1991 *A Dynamic Subgrid Scale Eddy Viscosity Model*. Physics of Fluids 3, 1760–1765.

[5] Germano M., Abbá A., Arina R. and Bonaventura L. 2014 *On the extension of the eddy viscosity model to compressible flows*. Physics of Fluids 26, 041702; doi: 10.1063/1.4871292.

[6] Hartel C., Meiburg E. and Necker F. 2000 *Analysis and direct numerical simulation of the flow at a gravity-current head. Part 1. Front topology and front speed for slip and non-slip boundaries*. Journal of Fluid Mechanics 418, 189–212.

[7] Hughes T.J.R., Feijoo G.R., Mazzei L. and Quincy J.B. 1998 *The variational multiscale method - a paradigm for computational mechanics*. Computer Methods in Applied Mechanics and Engineering 166, 3–24.

[8] Ooi S.K., Constantinescu G. and Weber L.J. 2007 *2D Large-Eddy Simulation of Lock-Exchange Gravity Current Flows at High Grashof Numbers*. Journal of Hydraulic Engineering 133, 1037–1047.

Derivation of an extended shallow water-Exner model with nonlocal solid discharge

Léa Boittin
Project-team ANGE, Inria; CEREMA; LJLL, UPMC Université Paris VI; UMR CNRS 7958
Inria, 2 rue Simone Iff - 75012 Paris, France
lea.boittin@inria.fr

Martin Parisot
Project-team ANGE, Inria; CEREMA; LJLL, UPMC Université Paris VI; UMR CNRS 7958
Inria, 2 rue Simone Iff - 75012 Paris, France
martin.parisot@inria.fr

Emmanuel Audusse
Université Paris 13; project-team ANGE, Inria
Université Paris 13, Institut Galilée, 99 avenue Jean-Baptiste Clément, 93430 Villetaneuse, France
audusse@math.univ-paris13.fr

Jacques Sainte-Marie
Project-team ANGE, Inria; CEREMA; LJLL, UPMC Université Paris VI; UMR CNRS 7958
Inria, 2 rue Simone Iff - 75012 Paris, France
jacques.sainte-marie@inria.fr

The simulation and prediction of sediment transport are relevant for environmental engineering purposes. Two transport modes exist: bedload transport, and suspended load transport. We deal here with the former. The Shallow Water-Exner system is commonly used to model it. However, this model does not have an associated energy, and it requires a closure relationship for the sediment discharge. We propose a new bedload transport model, deduced from a fluid description of the sediment layer.
We begin by focusing on a single sediment layer, and we intend to model its long-term evolution. This leads to the so-called diffusive limit of the Shallow Water equations. More precisely, our model is obtained by considering the balance between the pressure gradient and the dissipative forces. The system of PDEs thus derived presents a nonlocal solid discharge, namely

$$u_s = -(\kappa_B + \kappa - \nabla \cdot (\nu b \nabla^s \cdot))^{-1}(gb\nabla b - \kappa u_f),$$

where u_f is the velocity of the fluid layer above the sediment, b the thickness of the sediment layer, u_s its velocity, g the gravity acceleration, κ_B the bottom friction coefficient, κ the friction coefficient at the sediment-fluid interface and ν the kinematic viscosity. ∇^s denotes the symmetric gradient operator.
By degrading our equations in the inviscid case, an Exner-type model can be found. Nevertheless, in our opinion, the nonlocal effect is required to describe in a realistic manner the complex processes involved in sediment transport. The model has a dissipative energy equation, which allowed to conclude to the global well-posedness of the problem in a

simplified framework.
A numerical strategy for solving the system is presented. An asymptotic-preserving scheme is used. We compare the performances of our scheme with those of a classical scheme without asymptotic-preserving treatment. Finally, our simulations are compared with results obtained for granular flows.

Smoothed Particle Hydrodynamics Method for Multifluid Flow with Lava-Water Interaction

Vito Zago
Istituto Nazionale di Geofisica e Vulcanologia, sezione di Catania, Osservatorio Etneo
piazza Roma, 2 95125 - Catania Italy
vito.zago@ingv.it

Giuseppe Bilotta
Istituto Nazionale di Geofisica e Vulcanologia, sezione di Catania, Osservatorio Etneo
piazza Roma, 2 95125 - Catania Italy
giuseppe.bilotta@ingv.it

Annalisa Cappello
Istituto Nazionale di Geofisica e Vulcanologia, sezione di Catania, Osservatorio Etneo
piazza Roma, 2 95125 - Catania Italy
annalisa.cappello@ingv.it

Robert A. Dalrymple
Department of Civil Engineering, Johns Hopkins University, Baltimore, USA
201 Latrobe Hall, Baltimore, MD 21218.
rad@jhu.edu

Luigi Fortuna
Dipartimento di Ingegneria Elettrica Elettronica e Informatica, Universitá degli Studi di Catania, Italy
Via S. Sofia, 64 95123 - Catania Italy
luigi.fortuna@dieei.unict.it

Gaetana Ganci
Istituto Nazionale di Geofisica e Vulcanologia, sezione di Catania, Osservatorio Etneo
piazza Roma, 2 95125 - Catania Italy
gaetana.ganci@ingv.it

Alexis Hérault
Département Ingénierie Mathématique, Conservatoire des Arts et Metiers, Paris, France
292 Rue Saint-Martin, 75003 Paris, Francia
alexis.herault@cnam.fr

Ciro Del Negro
Istituto Nazionale di Geofisica e Vulcanologia, sezione di Catania, Osservatorio Etneo
piazza Roma, 2 95125 - Catania Italy
ciro.delnegalro@ingv.it

Smoothed Particle Hydrodynamics (SPH) [2] is a Lagrangian, meshless numerical method that has been recently gaining momentum in many applications of computational

fluid dynamics. In SPH a fluid is discretized with particles which are free to move with respect to each other. As the particles, which also act as interpolation nodes, are not bound to any given topological structure, SPH can easily manage fluids subject to large deformations, in contrast to traditional mesh-based numerical methods (such as finite differences, finite volumes, finite elements). Additionally, whereas mesh-based numerical methods often have to verify mass conservation, this is implicit in SPH, where mass is an intrinsic property of the particle. Likewise, front tracking is trivial in SPH, where surfaces (such as the free surface of the fluid, or solidification fronts) are implicitly defined by the particle position and thus automatically tracked. The motion of the particles in SPH, and the evolution of all of their properties (such as density and temperature), is driven by a discretization of the corresponding continuum equations (Navier-Stokes equations, continuity equation, heat equation). In its standard weakly-compressible formulation, the method is also easily parallelized, making it well-suited for implementation on modern high-performance computing hardware, such as GPUs. We present an application of GPUSPH, an implementation of the SPH method extended to include support for multiple fluids with different rheological properties, phase transition and temperature-dependent viscosity. The model is therefore extremely well-suited to study the emplacement of lava flows [1], a phenomenon which is characterized by free surfaces, irregular boundaries of natural topographies, as well as thermal dependency, including solidification and temperature-dependent viscosity. In this work we apply SPH to the study of the impact of lava/water interaction in the process of lava emplacement, modelling lava flowing into a water basin and comparing the resulting emplacement with the case of a dry environment with the same geometry, showing how the faster cooling due to the heat exchange affects the behavior of lava in the critical solidification phase.

References

[1] Bilotta, G., Hérault, A., Cappello, A., Ganci, G., Del Negro, C., *GPUSPH: a Smoothed Particle Hydrodynamics model for the thermal and rheological evolution of lava flows.* In: Harris, A. J. L., De Groeve, T., Garel, F. & Carn, S. A. (eds) Detecting, Modelling and Responding to Effusive Eruptions. Geological Society, London, Special Publications, 426, http://doi.org/10.1144/SP426.24

[2] Monaghan, J. J. 2005. *Smoothed Particle Hydrodynamics.* Reports on Progress in Physics, 68, 1703, http://doi.org/10.1088/0034-4885/68/8/R01

A Two-Layer Shallow-Water Type Model For Bedload Sediment Transport In Channels

Cipriano Escalante
Universidad de Málaga
Campus de Teatinos, s/n 29010 - Málaga Spain
escalante@uma.es

Enrique D. Fernández-Nieto
Universidad de Sevilla
Avda. Reina Mercedes, 2 41012 - Sevilla Spain
edofer@us.es

Tomás Morales de Luna
Universidad de Córdoba
Campus de Rabanales, 14071 - Córdoba Spain
tomas.morales@uco.es

Gladys Narbona-Reina
Universidad de Sevilla
Avda. Reina Mercedes, 2 41012 - Sevilla Spain
gnarbona@us.es

Two-layer models are commonly used in the literature to describe the bed-load phenomena in sediment transport problems (see [2, 4, 7]). Moreover, in that type of geophysical problems, the derivation of depth-integrated models −under the assumption of shallow flows− are extendedly accepted in order to get more manageable models that keep the essential effects. Thus, this type of models collects the different behavior of water and sediment from the dynamical point of view. By other hand, as it is pointed out in many works, the friction terms play an important role in this process, related to the exchange of mass and also to the relative movement of the two layers.

The known Saint-Venant-Exner model can then be seen as a simplification of a two-layer shallow-water model. In particular it is assumed a given discharge for the sediment layer, so the model for the bed-load transport reduces to a mass conservation equation.

In this work we present a two-layer shallow water model for bed-load sediment transport. Where, for the upper layer, we consider non-hydrostatic effects (see [1] and [6]).

The proposed model converges to a Saint-Venant-Exner type model when the velocity of the sediment layer is lower than the velocity of the fluid, or similarly, when the ratio between the hydrodynamic and the morphodynamic time is small (see [5]). Moreover, we proof that, by setting the definition of the friction forces, the solid transport discharge of the Saint-Venant-Exner model at which it converges can be prescribed. For example, we can set a configuration where the model converges to the generalization of the Meyer-Peter&Müller model proposed in [3].

Finally, the numerical approximation of the model and several numerical tests will be presented.

References

[1] M.O. Bristeau, A.Mangeney, J. Sainte-Marie, N. Seguin. 2015 *An energy-consistent depth-averaged Euler system: Derivation and properties.* Discrete and continuous dynamical system, 20, 961–988.

[2] E.D. Fernandez-Nieto, F. Bouchut, D. Bresch, M.J. Castro-Díaz, A. Mangeney, 2008. *A new Savage-Hutter type model for submarine avalanches and generated tsunami.* J. Comp. Phys., 227, 7720–7754.

[3] E.D. Fernández Nieto, T. Morales de Luna, G. Narbona-Reina, J.D. Zabsonré. 2016 *Formal deduction of the Saint-Venant-Exner model including arbitrarily sloping sediment beds and associated energy.* ESAIM: M2AN, doi:10.1051/m2an/2016018.

[4] L. Fraccarollo, H. Capart. *Riemann wave description of erosional dam-break flows.* J. Fluid Mech. 461, 183-228, (2002). DOI: 10.1017/S0022112002008455.

[5] G. Garegnani, G. Rosatti, L. Bonaventura. 2011 *Free surface flows over mobile bed: mathematical analysis and numerical modeling of coupled and decoupled approaches.* Applied And Industrial Mathematics, 2 (1).

[6] Y. Yamazaki, Z. Kowalik, K.F. Cheung. 2009 *Depth-integrated, non-hydrostatic model for wave breaking and run-up.* International Journal for Numerical Methods in Fluids, 61, 473–497.

[7] Y. Zech, S. Soares-Frazão, B. Spinewine, C. Savary, L. Goutière. *Inertia effects in bed-load transport models.* Can.J.Civ.Eng. 36, 1587–1597, (2009).

A two-phase model for fluidized granular flows with dilatancy effects and energy balance

Enrique D. Fernández-Nieto
Departamento de Matemática Aplicada I, Universidad de Sevilla
E.T.S. Arquitectura. Avda, Reina Mercedes, s/n. 41012 Sevilla, Spain
edofer@us.es

François Bouchut
Laboratoire d'Analyse et de Mathématiques Appliquées
LAMA - UMR 8050. Université Paris-Est - Marne-la-Vallée, France
francois.bouchut@univ-mlv.fr

El Hadji Koné
Institut de Physique du Globe de Paris, Equipe de Sismologie.
1 rue Jussieu, 75005 Paris, France
kone@ipgp.fr

Anne Mangeney
Université Paris Diderot, Sorbone Paris Cité, Institut de Physique du Globe de Paris
Equipe de Sismologie. 1 rue Jussieu, 75005 Paris, France
mangeney@ipgp.jussieu.fr

Gladys Narbona-Reina
Departamento de Matemática Aplicada I, Universidad de Sevilla
E.T.S. Arquitectura. Avda, Reina Mercedes, s/n. 41012 Sevilla, Spain
gnarbona@us.es

In this talk a two-phase/two-thin-layer model for fluidized debris flows is presented. It takes into account the compression/dilatation of the granular media and its interaction with the pore fluid pressure, and verifies an energy balance (see [2]).

The model is derived from a 3D two-phase Jackson's model [4]. This system has 5 unknowns: the solid and fluid velocities, the solid and fluid pressures and the solid volume fraction. As a result, an additional equation inside the mixture is necessary to close the system. Surprisingly, this issue is inadequately accounted for in the models that have been developed on the basis of JacksonÕs work (see [1]).

We present in this talk (see [2]), an approach to correctly deal with the thermodynamics of JacksonÕs model by closing the mixture equations by a weak compressibility relation following [7]. This relation implies that the occurrence of dilation or contraction of the granular material in the model depends on whether the solid volume fraction is respectively higher or lower than a critical value. When dilation occurs, the fluid is sucked into the granular material, the pore pressure decreases and the friction force on the granular phase increases. On the contrary, in the case of contraction, the fluid is expelled from the mixture, the pore pressure increases and the friction force diminishes. To account for this transfer of fluid into and out of the mixture, a two-layer model is proposed with a

fluid layer on top of the two-phase mixture layer. Mass and momentum conservation are satisfied for the two phases, and mass and momentum are transferred between the two layers. A thin-layer approximation is used to derive average equations. Special attention is paid to the drag friction terms that are responsible for the transfer of momentum between the two phases and for the appearance of an excess pore pressure with respect to the hydrostatic pressure.

Finally, we present several numerical tests by comparing with the models proposed in [5] and [3], and with experimental data.

References

[1] F. Bouchut, E.D. Fernandez-Nieto, A. Mangeney, G. Narbona-Reina, 2015 *A two-phase shallow debris flow model with energy balance*. ESAIM: Math. Modelling Num. Anal., 49, 101–140.

[2] F. Bouchut, E. D. Fernandez-Nieto, A. Mangeney, G. Narbona-Reina, 2016 *A two-phase two-layer model for fluidized granular flows with dilatancy effects* J. Fluid Mech., accepted for publication.

[3] R. M. Iverson and D. L. George, 2014 *A depth-averaged debris-flow model that includes the effects of evolving dilatancy. I. Physical basis*. Proc. R. Soc. A, 470:20130819.

[4] R. Jackson, 2000 *The Dynamics of Fluidized Particles*. Cambridges Monographs on Mechanics.

[5] M. Pailha and O. Pouliquen, 2009 *A two-phase flow description of the initiation of underwater granular avalanches*. J. Fluid Mech., 633:115Ð135.

[6] E.B. Pitman, L. Le, 2005 *A two-fluid model for avalanche and debris flows*. Phil.Trans. R. Soc. A, 363, 1573–1601.

[7] S. Roux, F. Radjai, 1998 *Texture-dependent rigid plastic behaviour*. Proceedings: Physics of Dry Granular Media, September 1997. (eds. H. J. Herrmann et al.). Kluwer. Cargèse, France, 305–311.

Toy models of frazil ice formation in turbulent overcooled water

Piero Olla
ISAC-CNR and INFN, Sez. Cagliari
I-09042, Cagliari, Italy
olla@dsf.unica.it

Francesca De Santi
ISAC-CNR and INFN, Sez. Cagliari
I-09042, Cagliari, Italy
fdesanti@dsf.unica.it

Ice production in polar oceans usually occurs in the presence of turbulence and wave motions induced by strong winds. This prevents the formation of a continuous ice layer at the sea surface (thin ice films, called nilas, are indeed observed in very calm conditions). A slurry of ice crystals, with a characteristic milky or greasy appearance, is generated instead. The ice crystals, called frazil crystals or frazil ice, have diameters ranging from 0.01 up to ~ 4 mm and thickness from 1 to 100 μm [1]. If the wind is sufficiently strong, the frazil ice may be blown away, leaving the water surface exposed to the cold air, thus enhancing the ice production and the heat transfer to the atmosphere [2].
We can list the most important phenomena expected to contribute to frazil ice formation.

- Small droplets and foam are continuously lifted up from the water surface and freeze in contact of the cold air. When they return to the water column they act as primary congelation seeds.
- If the upper layers of the ocean are sufficiently overcooled, ice crystals grow out of the congelation seeds and reach size up to the millimeter range. New seeds are generated through fragmentation induced by collisions with other crystals (secondary nucleation).
- Part of the crystals are entrained by the turbulence and are transported down the column. Additional ice production may take place away from the surface if the overcooling is sufficient. Field data indicate that underwater frazil ice and significant overcooling in the water column may indeed be present down to depths of 20–40 m.

Due to the complexity of the processes involved, models of frazil ice formation necessarily rely on parameterization of small scale phenomena and on the introduction of empirical constants. In such circumstances, it may be of some interest to take a different approach, and look for limit regimes in which a reduced number of parameter is at play and identification of key physical aspects is simpler.
We focus on a stationary regime in which the ice formation process can be described as a balance of fluxes, as illustrated in Fig. 1. During freezing, most of the salt in forming the crystals will be released in the environment together latent heat. The freezing temperature T_i is a decreasing function of the salinity deviation S,

$$T_i = T_{iB} - a_S S, \qquad a_S \simeq 0.0573 \ ^{\circ}\mathrm{C/psu}, \tag{1}$$

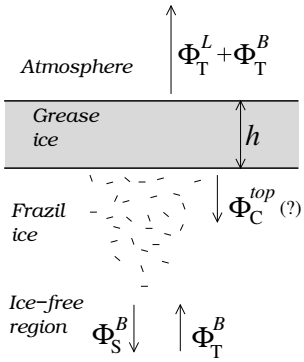


Figure 1: Sketch of the heat, salinity and ice fluxes generated during build-up of a grease ice layer. The heat flux to the atmosphere is split into latent heat Φ_T^L and sensible heat Φ_T^B contributions. The salinity flux Φ_S^B is downward directed. The question mark indicates that the sign of the frazil ice flux Φ_C^{top} is a priori undetermined.

where $T_{iB} \simeq -2.09$°C is the freezing temperature at a reference salinity $S_B = 34.5$ psu. Ice production thus contributes to reduction of the overcooling

$$T_o = T - T_{iB} + a_S S \tag{2}$$

both through latent heat production and salt release, even though latent heat turns out to dominate. On the other hand, it is possible to see that salinity contribution to buoyancy greatly exceeds that from latent heat release. In a situation in which ice forms mainly at the water surface, a fraction of the order of 1/10 of the heat flux to the atmosphere coming from ice formation would produce a salinity flux in the water column whose effect in terms of convection would dominate that of the heat flux.
An assumption of overcooling decreasing with depth (T_o becoming more negative approaching the water surface) is sufficient to impose interesting conditions on the ratio of sensible to latent heat flux to the atmosphere. Indicating with Π_C the ice formation rate at the surface, with Φ_T^L the latent heat contribution to the heat flux, and with Φ_S the salinity flux, we have

$$-\Phi_S/S_B = \Phi_T^L/\hat{\mathcal{L}} = \Pi_C, \tag{3}$$

where $\hat{\mathcal{L}} \simeq 75.5$ °C is the temperature increase from latent heat release in an volume of water equal to that undergoing freezing. Imposing $T_o' < 0$ (z upward directed) implies an analogous condition for the overcooling flux in the water column: $\Phi_{T_o} = \Phi_T^B + a_S S > 0$. On the other hand, Eq. (3) allows to write for the total heat flux $\Phi_T^{tot} = \Phi_T^B - (\hat{\mathcal{L}}/S_B)\Phi_S$, which gives a minimum for the sensible to total heat flux ratio $\mathcal{B} = \Phi_T^B/\Phi_T^{tot}$:

$$\mathcal{B}_{min} = \frac{a_S S_B}{\hat{\mathcal{L}} + a_S S_B} \simeq 0.025. \tag{4}$$

An important question concerns the amount of ice produced far from the water surface. Such contribution should clearly be taken into account in the presence of overcooling reaching to sufficient depth. Also in this case a stationary hypothesis allows us to describe the dynamics in terms of a balance of fluxes. The change of the overcooling flux Φ_{T_o} in passing from the frazil ice rich region on top of the column to the frazil ice free bottom is

$$\Phi_{T_o}^B = \Phi_{T_o}^{top} - (\hat{\mathcal{L}} + a_S S_B)\Phi_C^{top}, \tag{5}$$

where Φ_C is the ice flux expressed in terms of the ice volume fraction field C. The contribution $-(\hat{\mathcal{L}} + a_S S_B)\Phi_C^{top}$ is precisely the latent heat ceded by the water phase upon melting of the crystals.
Estimates of the fluxes can be obtained considering that frazil ice forms in windy conditions such that a mechanical boundary layer is expected at the top of the water column. A wind speed of the order of 10 m/s and a total heat flux to the atmosphere of the order of 1 kW/m^2 would give an Obukhov depth of the order of 3 m. Smaller heat fluxes and stronger winds, which would lead to larger Obukhov depths, are however to be expected. We will show how such estimates could be obtained in terms of just two parameters that are the entrainment rate of the frazil crystals in the water column

$$\mathcal{E} = -(\hat{\mathcal{L}} + a_S S_B)\Phi_C^{top}/\Phi_{T_o}^B, \tag{6}$$

and the ratio $\mathcal{B}$ which determines the ratio between depth λ of the region in which transport dominates over destruction by ice formation dominates the overcooling, and the Obukhov depth L_S

$$\lambda/L_S \simeq \frac{\sigma\alpha_S S_B}{\mathcal{B}u_*\gamma\hat{\mathcal{L}}}, \tag{7}$$

where the parameters entering the above formula are, respectively: $\sigma \simeq 0.4$ the von Karman constant; $\alpha_S \simeq 7.7 \cdot 10^{-3}$ m/(psu s^2) the haline buoyancy coefficient; u_* the friction velocity (for a wind velocity of 10 m/s at 10 m from the water surface, $u_* \approx 1$ cm/s); γ the ice formation rate (current estimates give $\gamma \approx 0.003$ (^{o}C s)$^{-1}$ [3, 4]).

References

[1] S. Martin, Frazil ice in rivers and oceans. Ann. Rev. Fluid Mech. **91** (1981) 756

[2] A. Alam and J.A. Curry, Evolution of new ice and turbulent fluxes ove freezing winter leads. J. Geophys. Res. **103**C (1998) 15783

[3] L. Hammar and H.T. Shen, Frazil evolution in channels. J. Hydraul. Res. **33** (1995) 291

[4] P.R. Holland, D.L. Feltham and S. Daly, On the Nusselt number for frazil ice growth a correction to Frazil evolution in channels by Lars Hammar and Hung-Tao Shen. J. Hydraul. Res. **45** (2007) 421

Inverse problems and control of PDEs

PROPOSERS

Piermarco Cannarsa
Università degli Studi di Roma "Tor Vergata"
Via della Ricerca Scientifica 1, 00133 - Roma Italy
cannarsa@mat.uniroma2.it

Giuseppe Floridia
Università degli Studi di Napoli Federico II
Via Cintia, Monte S. Angelo, I-80126 - Napoli, Italy
giuseppe.floridia@unina.it

SPEAKERS

Michel Cristofol
CMI, Universitè Aix-Marseille
michel.cristofol@univ-amu.fr

Sylvain Ervedoza
Institut de Mathématiques de Toulouse, Université Paul Sabatier Toulouse III
ervedoza@math.univ-toulouse.fr

Emanuele Haus
Dip. di Matematica e Applicazioni "R. Caccioppoli", Università degli Studi di Napoli Federico II
emanuele.haus@unina.it

Gianluca Mola
Dip. di Matematica, Politecnico di Milano
gianluca.mola@polimi.it

Alessio Porretta
Dip. di Matematica, Università degli Studi di Roma "Tor Vergata"
porretta@mat.uniroma2.it

Masahiro Yamamoto
Department of Mathematical Sciences, University of Tokyo
myama@next.odn.ne.jp

In the applied sciences, one is often by the need to reconstruct some parameter appearing in differential models from appropriate measurements of the solutions (see, e.g., [3]). In mathematical terms, these issues lead to inverse problems for partial differential equations (PDE's) and will be the main subject of this minisymposium. In contrast to forward problems, inverse problems are typically ill-posed. On the other hand, some of the techniques which are commonly used to investigate stability, unique continuation, and controllability for PDE's have proven to be crucial in the study of inverse problems. A case in point is represented by Carleman estimates, that can be applied to derive observability inequalities as well as Lipschitz stability estimates ([1, 2]). Topics to be

discussed in this minysimposium also include interior or boundary trace regularity result, stability properties, and decay rates of solutions in the case of dissipative evolutionary equations.

References

[1] Beauchard, K., Cannarsa, P. and Yamamoto M. 2014 *Inverse source problem and null controllability for multidimensional Grushin-type parabolic operators*, Inverse Probl. 30, (2), 26 p.

[2] Cannarsa, P., Martinez, P. and Vancostenoble, J. 2016 *Global Carleman estimates for degenerate parabolic operators with applications*, in, Memoirs of the AMS, vol. 239, Amer. Math. Soc., Providence, RI, 1–209.

[3] Roques, L. and Cristofol, M. 2010 *On the determination of the nonlinearity from localized measurements in a reaction-diffusion equation.* Nonlinearity 23 (3), 675–686.

A pointwise measurements method for some parabolic problems

Michel Cristofol
Université d'Aix-Marseille
Institut de Mathématiques de Marseille, UMR CNRS 7373, Ecole Centrale, 13288 - Marseille, France
michel.cristofol@univ-amu.fr

How to get uniqueness using as less as possible of observations ? Basing my talk around a toy problem : reconstruction of the potential for a linear parabolic problem, I will recall two classical methods : Dirichlet to Neumann map (DtN) [1] and Carleman estimates [6]. Then I will present a different and Êrecent approach based on pointwise observations [4, 2, 5, 3] and I will underline some points to be improved for each method. Then, I will end my talk by a review of some results related to this pointwise observations method.

References

[1] Choulli M, 2009 *Une introduction aux problemes inverses elliptiques et paraboliques.* Springer.

[2] Cristofol M, Garnier J, Hamel F and Roques L . 2011 *Uniqueness from pointwise observations in a multiparameter inverse problem.* Commun. Pure Appl. Anal. 11 1Ð15

[3] Roques L, Chekroun R D, Cristofol M, Soubeyrand S and Ghil M . 2014 *Parameter estimation for energy balance models with memory.* Proc. R. Soc. A 470

[4] Roques, L and Cristofol, 2010 *On the determination of the nonlinearity from localized measurements in a reactionÐdiffusion equation.* Nonlinearity 23 675Ð86

[5] Roques l and Cristofol M . 2012 *The inverse problem of determining several coefficients in a nonlinear LotkaÐVolterra system.* Inverse Problems 28 075007 12pp

[6] Yamamoto M, 2009 *Carleman estimates for parabolic equations and applications.* Inverse Problems 25 123013 75 pp

On the reachable set of the heat equation

Sylvain Ervedoza
Institut de Mathématiques de Toulouse & CNRS
Université Paul Sabatier, Toulouse, France
sylvain.ervedoza@math.univ-toulouse.fr

Jérémi Dardé
Institut de Mathématiques de Toulouse
Université Paul Sabatier, Toulouse, France
jeremi.darde@math.univ-toulouse.fr

The goal of this talk is to present a new result concerning the reachable set of the heat equation in space dimension 1. Our approach characterizes the target states in terms of the set on which an analytic expansion exists. To be more precise, when considering the heat equation on a space interval $(-L, L)$ and controlled from both boundaries $x = -L$ and $x = L$, we show that a function $y = y(x)$ belongs to the reachable set when it admits an analytic extension in a square of the form $\{z = x_1 + \mathbf{i}x_2 \text{ with } |x_1| + |x_2| \leq L'\}$ for some $L' > L$. This result is mainly sharp as one can show that a reachable state necessarily admits an analytic extension in $\{z = x_1 + \mathbf{i}x_2 \text{ with } |x_1| + |x_2| \leq L\}$. Our approach is based on a suitable "limiting" Carleman estimate for the heat equation and suitable duality properties.
Let us finally note that this result improves previous ones, namely [2], [1], and [3] which was the first work considering the characterization of the reachable states through the set where they admit an analytic extension.

References

[1] S. Ervedoza and E. Zuazua. Sharp observability estimates for heat equations. *Arch. Ration. Mech. Anal.*, 202(3):975–1017, 2011.

[2] H. O. Fattorini and D. L. Russell. Exact controllability theorems for linear parabolic equations in one space dimension. *Arch. Rational Mech. Anal.*, 43:272–292, 1971.

[3] P. Martin, L. Rosier, and P. Rouchon. On the reachable sets for the boundary control of the heat equation. *Applied Mathematics Research eXpress*, 2016.

Exact Controllability for Quasi-Linear Perturbations of KdV

Emanuele Haus
Università di Napoli Federico II - Dipartimento di Matematica e Applicazioni "R. Caccioppoli"
via Cintia - Monte Sant'Angelo - 80126 Napoli (Italy)
emanuele.haus@unina.it

Pietro Baldi
Università di Napoli Federico II - Dipartimento di Matematica e Applicazioni "R. Caccioppoli"
via Cintia - Monte Sant'Angelo - 80126 Napoli (Italy)
pietro.baldi@unina.it

Giuseppe Floridia
Università di Napoli Federico II - Dipartimento di Matematica e Applicazioni "R. Caccioppoli"
via Cintia - Monte Sant'Angelo - 80126 Napoli (Italy)
giuseppe.floridia@unina.it

We prove that the KdV equation on the circle remains exactly controllable in arbitrary time with localized control, for sufficiently small data, also in presence of quasi-linear perturbations, namely nonlinearities containing up to three space derivatives, having a Hamiltonian structure at the highest orders. We use a procedure of reduction to constant coefficients up to order zero (adapting [1]), classical Ingham inequality and HUM method to prove the controllability of the linearized operator. Then we prove and apply a modified version of the Nash-Moser implicit function theorem by Hörmander [2].

References

[1] P. Baldi, M. Berti, R. Montalto, *KAM for quasi-linear and fully nonlinear forced perturbations of Airy equation*. Math. Annalen 359 (2014), 471-536.

[2] L. Hörmander, *On the Nash-Moser implicit function theorem*. Ann. Acad. Sci. Fenn. Ser. A I Math. 10 (1985), 255-259.

On the identification of constant coefficients in a model of linear anisotropic diffusion

Gianluca Mola
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
gianluca.mola@polimi.it

Let $(H, \langle \cdot, \cdot \rangle)$ be a complex Hilbert space and $A_i : D(A) \to H$ $(i = 1, \cdots, n)$ be a family of nonnegative and self-adjoint operators. We study the inverse problem consisting in the identification of the function $u : [0, T] \to H$ and n constants $\alpha_1, \cdots, \alpha_n > 0$ (*diffusion coefficients*) that fulfill the initial-value problem

$$u'(t) + \alpha_1 A_1 u(t) + \cdots + \alpha_n A_n u(t) = 0, \quad t \in (0, T), \quad u(0) = x,$$

and the additional conditions

$$\langle A_1 u(T), u(T) \rangle = \varphi_1, \quad \cdots \quad , \langle A_n u(T), u(T) \rangle = \varphi_n.$$

Under suitable assumptions on the operators A_i and on the data $x \in H$ and $\varphi_1, \cdots, \varphi_n > 0$, we shall prove that the solution of such a problem is unique and depends continuously on the data. Applications are considered.

This extends previous results achieved by the author in the cases when $n = 1$ ([2] and [4]) and $n = 2$ ([1] and [3]).

References

[1] Lorenzi, L. and Mola, G. 2012 *Recovering the reaction and the diffusion coefficients in a linear parabolic equation*, Inverse Problems **28**.

[2] Mola, G. 2011 *Identification of the diffusion coefficient in linear evolution equations in Hilbert spaces*, J. Abstract Differential Equations and Applications **2** , vol. 1, pp. 14–28.

[3] Mola, G., Okazawa, N. and Yokota, T. 2016 *Reconstruction of two constant coefficients in linear anisotropic diffusion model*, submitted.

[4] Mola, G., Okazawa, N., Prüss, J. and Yokota, T. 2011 *Semigroup-theoretic approach to identification of linear diffusion coefficients*, Discrete Continuous Dynamical Systems, Series S **9**, No. 3, pp. 777 - 790.

On the turnpike property in optimal control systems

Alessio Porretta
Università degli Studi di Roma Tor Vergata
Via della Ricerca Scientifica 1, 00133 - Roma, Italy.
porretta@mat.uniroma2.it

We discuss the behavior of optimal control problems in a long horizon $(0, T)$ and the so-called turnpike property, which means that the optimal control and trajectory are close to the corresponding stationary optima for most of the time, far from initial and final time. This is an evidence of robustness of the cost criterion, leading to optima profiles which are mostly independent of initial data and terminal pay-off. In joint works with E. Zuazua, we analyze this property for linear quadratic control problems in finite and infinite dimension showing the role played by stabilization (as well as observability and controllability) in this kind of question and proving that the proximity between time-dependent and stationary optima holds with exponential rate.

Inverse Problems of Determining Moving Sources in Wave Equation and Heat Equation

Masahiro Yamamoto
The University of Tokyo
3-8-1 Komaba Meguro Tokyo 153-8914 Japan
myama@ms.u-tokyo.ac.jp

Let $\Omega \subset \mathbb{R}^n$ be a bounded domain with smooth boundary $\partial\Omega$. We consider

$$\begin{cases} \partial_t^2 u = \Delta u + f(x - \alpha(t)), \quad x \in \Omega,\ -T < t < T, \\ u|_{\partial\Omega} = 0, \\ u(x,0) = \partial_t u(x,0) = 0, \quad x \in \Omega. \end{cases} \tag{1}$$

and

$$\begin{cases} \partial_t u = \Delta u + f(x - \alpha(t)), \quad x \in \Omega,\ -T < t < T, \\ u|_{\partial\Omega} = 0, \\ u(x,0) = 0, \quad x \in \Omega. \end{cases} \tag{2}$$

Here $\alpha(t) = (\alpha_1(t), ..., \alpha_n(t))$. Let $\omega \subset \overline{\Omega}$ be a domain such that $\overline{\omega} \supset \partial\Omega$ and $T > 0$ be given. Then we consider the following two types of inverse problems.

- **Inverse Problem I.**
  Determination of a shape f of a moving source by data $u|_{\omega\times(-T,T)}$ provided that the orbit $\alpha(t)$, $-T \le t \le T$, is known.
- **Inverse Problem II.**
  Determination of an orbit $\alpha(t)$ of a moving source by data $u|_{\omega\times(-T,T)}$ provided that the shape $f(x)$, $x \in \Omega$, is known.

We will present the uniqueness and some conditional stability for the two kinds of inverse problems for the wave and the heat equations. We will describe the uniqueness result for the inverse problem of determining $f(x)$ in (1). We assume and define:

$$\alpha(0) = 0, \quad \|\alpha''\|_{C[-T,T]} + \|\alpha^{(3)}\|_{C[-T,T]} \le M, \tag{3}$$

there exist constants $\delta > 0$ and $x_0 \in \mathbb{R}^n \setminus \overline{\Omega}$ such that

$$\cos\angle(\alpha(t), x - x_0) \le -\delta, \quad x \in \overline{\Omega},\ -T \le t \le T, \quad 2\delta \min_{x\in\overline{\Omega}} |x - x_0| > \|\alpha\|_{C[-T,T]} \tag{4}$$

and for arbitrarily fixed $M \ge 0$ we assume that

$$f \in \mathcal{F} := \{f \in C^1(\mathbb{R}^n);\ \text{supp } f \text{ is compact and there exists}$$

$$\text{a constant } C > 0 \text{ such that} \quad M|\nabla f(x)| \le C|f(x)|, \quad x \in \mathbb{R}^n\}. \tag{5}$$

The second condition in (4) can be satisfied if x_0 is sufficiently far away from Ω, while the first condition means that the orbit should be included in some range of directions from the origin.

Example Let $\alpha(t) = ct$ with $c \in \mathbb{R}^n, \neq 0$. In (3) we can choose $M = 0$. In (4) we can choose $x_0 \in \mathbb{R}^n \setminus \overline{\Omega}$ such that $\cos \angle(c, x - x_0) < 0$ for $x \in \overline{\Omega}$, because $\alpha(t)$ has one fixed direction, and since we can set $M = 0$ in (5), we have $\mathcal{F} = C^1(\overline{\Omega})$.
The set $\mathcal{F}$ is an admissible set of unknown f and for general $\alpha(t)$, the set is quite restrictive. We have

Example for $\mathcal{F}$. Let $\psi_k \in C_0^1(\mathbb{R}^n)$, $k = 1, 2, ..., N$ be linearly independent on $\overline{\Omega}$ and satisfy $\psi_k > 0$ on $\overline{\Omega}$. Then

$$\left\{ f = \sum_{k=1}^{N} a_k \psi_k;\ a_1, ..., a_N \geq 0 \right\}$$

satisfies (5). This is a subset in $\mathbb{R}^N$ and so our inverse problem in this case is the determination of a finite number $a_1, ..., a_N$ of real numbers. Then we can state the uniqueness for Inverse Problem I for (1).
We assume

$$T > \max_{x \in \overline{\Omega}} |x - x_0|.$$

In (1), if $u|_{\omega \times (-T,T)} = 0$, *then* $f = 0$ *in* Ω.

This is a joint work with Professor Piermarco Cannarsa (Univ. Roma "Tor Vergata").

Modeling Dissipative Phenomena - Part I: Damage and viscoelasticity

PROPOSERS

Maurizio Grasselli
Politecnico di Milano
P.zza Leonardo da Vinci, 32 20133 - Milano - Italy
maurizio.grasselli@polimi.it

Elena Bonetti
Università degli Studi di Milano

Cecilia Cavaterra
Università degli Studi di Milano

Monica Conti
Politecnico di Milano

SPEAKERS

Monica Conti
Politecnico di Milano
monica.conti@polimi.it

Filippo Dell'Oro
Politecnico di Milano
filippo.delloro@polimi.it

Francesco Freddi
Università degli Studi di Parma
francesco.freddi@unipr.it

Andrei Constantinescu
CNRS - Ecole Polytechnique, Paris
andrei.constantinescu@lms.polytechnique.fr

Riccarda Rossi
Università degli Studi di Brescia
riccarda.rossi@unibs.it

Giulia Scalet
Università degli Studi di Pavia
giulia.scalet@unipv.it

Dissipation of energy is ubiquitous in Nature. Damage, viscoelasticity, phase changes are just some important examples of such phenomena. They are all characterized by an energy which decreases over time. The goal of this minisymposium is to present an up-to-date overview of their mathematical treatment. The minisymposium is divided into two parts. The first is devoted to mathematical models of damaging, fatigue, aging

and viscoelasticity. All these phenomena are related to a losing of elastic response of materials, which may decrease in time or due to the damaging of internal cohesion bonds. The second is concerned with diffuse interface models which have recently received a lot of attention since they can be employed to describe a large variety of phenomena. In particular, we recall phase separation, tumor growth, image inpainting and liquid crystals.

A Mathematical Model for Aging Viscoelastic Materials

Monica Conti
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
monica.conti@polimi.it

Valeria Danese
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
valeria.danese@polimi.it

Claudio Giorgi
Università di Brescia - DICATAM
Via Valotti, 9 25133 Brescia Italy
giorgi@ing.unibs.it

Vittorino Pata
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
vittorino.pata@polimi.it

We propose a mathematical model for the analysis of aging phenomena (or, more generally, changes of the structural properties) of a viscoelastic material within the dynamics. The model is in the form of an integro-differential equation

$$u_{tt} - h_t(0)\Delta u - \int_0^\infty h_t'(s)\Delta u(t-s)ds + f(u) = g,$$

where, the main feature is that the memory kernel $h_t(\cdot)$ depends on time. A proper notion of solution and a global well-posedness result are discussed in the newly established framework of dynamical systems acting on time-dependent spaces [1, 2].

References

[1] M. Conti, V. Pata, R. Temam 2013 *Attractors for processes on time-dependent spaces. Applications to wave equations*, J. Differential Equations 255, 1254–1277

[2] F. Di Plinio, G.S. Duane, R. Temam 2011 *Time dependent attractor for the oscillon equation*, Discrete Contin. Dyn. Syst. 29, 141–167

The Moore-Gibson-Thompson equation with memory in the critical case

Filippo Dell'Oro
Politecnico di Milano
Via Bonardi 9, 20133 Milano, Italy
filippo.delloro@polimi.it

Irena Lasiecka
University of Memphis - Department of Mathematical Sciences
Memphis, TN, 38152, USA
lasiecka@memphis.edu

Vittorino Pata
Politecnico di Milano
Via Bonardi 9, 20133 Milano, Italy
vittorino.pata@polimi.it

We consider the following abstract version of the Moore-Gibson-Thompson equation with memory

$$\partial_{ttt}u(t) + \alpha\partial_{tt}u(t) + \beta A\partial_t u(t) + \gamma Au(t) - \int_0^t g(s)Au(t-s)\mathrm{d}s = 0$$

depending on the parameters $\alpha, \beta, \gamma > 0$, where A is strictly positive selfadjoint linear operator and g is a convex (nonnegative) memory kernel. In the subcritical case $\alpha\beta > \gamma$, the related energy has been shown to decay exponentially in [1]. Here we discuss the critical case $\alpha\beta = \gamma$, and we prove that exponential stability occurs if and only if A is a bounded operator. Nonetheless, the energy decays to zero when A is unbounded as well.

References

[1] Lasiecka, I. and Wang, X. 2016 *Moore-Gibson-Thompson equation with memory, part I: Exponential decay of energy.* Z. Angew. Math. Phys. 67, n.17

Variational cohesive fracture mechanics: numerical assessment

Francesco Freddi
Università degli Studi di Parma
Parco Area delle Scienze, 181/A 43124 - Parma Italy
francesco.freddi@unipr.it

Flaviana Iurlano
Universität Bonn
Piazza Leonardo da Vinci, 32 53115 - Bonn Germany
iurlano@iam.uni-bonn.de

Cohesive models in Fracture Mechanics are based on the idea that fracture energy is gradually released with the growth of the crack opening, reflecting the progressive weakening of the bound between the lips [3]. In contrast, in the brittle model of Griffith the fracture energy is instantaneously dissipated at crack initiation.
In the last years fracture problems have been revisited taking advantage of tools and techniques from calculus of variations [4], so that a consistent and rigorous treatment of the matter, although with some limit, arose. The main drawback of this approach runs over numerical implementations, which has been overcome with a regularized version of the fracture model, and precisely a phase-field model.
Phase-field models have recently found widespread popularity for simulating brittle crack propagation in a smeared manner [5, 10]. The analytical substrate is the Γ-convergence result by Ambrosio and Tortorelli [1], which gives the convergence of global minima. We also remark that a number of phenomena that are difficult to capture in discrete crack models, like crack branching, can evolve naturally in a phase-field approach.
The counterpart of [2] in the cohesive context is represented by the recent work [7]. In this paper, fully detailed in [9], we aim to simulate cohesive crack propagation using the smeared models introduced in [7]. Using alternate minimization technique and backtracking algorithm we reconstruct the Barenblatt's cohesive energy and the stress-crack opening law in a 1D traction experiment. It is interesting to notice that without backtracking procedure such curves get close to those corresponding to the homogeneous solution at moderate opening.
Irreversibility is quite a controversial issue in cohesive context and its discussion goes out of the aims of the present work. We refer to [6, 8] for a comprehensive analysis and a discussion of the relevant issues. Here we assume the standard damage irreversibility on the smeared functionals by requiring the monotonicity of the damage variable. It turns out that the stress-crack opening law is linear during unloading and reloading up to the maximal opening, where we recover the standard Barenblatt's law.
We also consider a fully regularized version of the phase-field models [7] and we compare its behavior with the previous one. Finally, this formulation turns out to be effective in 2D experiments, for which no theoretical results are currently available. We briefly recall the formulation and illustrate a simple 1D numerical example.

1 Formulation

Let $\Omega \subset \mathbb{R}^d$ be a bounded open set with Lipschitz boundary representing the crack-free reference configuration of an elastic body. We assume that, due to suitable external forces and boundary conditions, the body undergoes a crack along a $(d-1)$-dimensional manifold $M \subset \Omega$ and a displacement u on $\Omega \setminus M$.
In the classical cohesive model, the evolution of the crack is governed by an energy which is the sum of a bulk term, the energy of the crack-free part, and of a surface term, the energy spent to separate fracture lips. The former depends on the strain, the latter on the crack set and amplitude, through an appropriate density $g : \mathbb{R} \to [0, +\infty]$.
The variational formulation of the model involves the space of (generalized) functions with bounded variation $(G)BV$. Then the stationary cohesive fracture energy in case of antiplane shear reads as

$$\mathcal{F}(u) := \int_\Omega \psi(|\nabla u|)dx + \int_{J_u} g(|[u]|)d\mathcal{H}^{d-1} + \sigma_c\,|D^c u|(\Omega), \tag{1}$$

where $u \in GBV(\Omega)$, ψ is quadratic near the origin and asymptotically linear, g is nondecreasing, concave, bounded, $g(0) = 0$, the slope of g in 0 is $\sigma_c \in (0, +\infty)$. The last term in (1) can be interpreted as a micro-crack energy.
Note that in 1D, under suitable hypotheses on ψ, g, boundary conditions, and forces, a global minimizer $\overline{u}$ of (1) belongs to SBV and $\psi(\overline{u}) = \overline{u}^2$.
Let us now introduce the variational approximation of (1) obtained in [7, Theorem 3.1]. For definition and properties of Γ-convergence we refer to [8]. Given two infinitesimal sequences $0 < \eta_\delta << \delta$ and $c, \gamma \in (0, +\infty)$, we consider the functionals F_δ defined by

$$F_\delta(u, v) := \int_\Omega \left(\frac{c}{2}(\eta_\delta + f_\delta^2(v))|\nabla u|^2 + \gamma \left(\frac{(1-v)^2}{4\delta} + \delta|\nabla v|^2 \right) \right) dx \tag{2}$$

for $(u, v) \in H^1(\Omega)\times H^1(\Omega)$ and $0 \le v \le 1$ a.e., and by $+\infty$ otherwise in $L^1(\Omega)\times L^1(\Omega)$, where

$$f_\delta(z) := 1 \wedge \delta^{1/2}\frac{z}{1-z}\,, \qquad f_\delta(1) := 1. \tag{3}$$

By [7, Theorem 3.1] as $\delta \to 0$ the functionals F_δ Γ-converge in $L^1(\Omega)\times L^1(\Omega)$ to the functional $F(u, v) := \mathcal{F}(u)$ defined in (1), if $u \in GBV(\Omega)$ and $v = 1$ a.e., $F(u, v) := +\infty$ elsewhere. The surface density g is given by the following one-dimensional minimum problem

$$g(s) := \inf_{(\alpha,\beta)} \int_0^1 \sqrt{\frac{c\gamma}{2}\beta^2|\alpha'|^2 + \gamma^2(1-\beta^2)|\beta'|^2}\,dr, \tag{4}$$

where $\alpha, \beta \in H^1\big((0,1)\big)$ satisfy $0 \le \beta \le 1$, $\alpha(0) = 0$, $\alpha(1) = s$, $\beta(0) = \beta(1) = 1$. In particular g is nondecreasing, subadditive, $g(0) = 0$, the slope of g in 0 is $\sigma_c := (c\gamma/2)^{1/2}$, and the asymptotic limit as $s \to +\infty$ is γ; moreover $\psi(s) := cs^2/2$ for $s \le (\gamma/(2c))^{1/2}$ and $\psi(s) := \sigma_c s - \gamma/4$ elsewhere (see [7, Proposition 4.1]).

2 Numerical example

As an example in the following, we describe the evolutionary solution to the traction problem for a one-dimensional homogeneous bar obtained by FEM approximation of the functional (2). Full details can be found in [9].
Let $\Omega := [0, L]$, so that $\partial\Omega = \{0, L\}$. We follow the evolution in the time interval

$[0, T] = [0, 1]$, assuming that the left extremity at $x = 0$ is clamped, while a displacement $u = u_0\, t$ is imposed at $x = L$. Here u_0 is a reference length and $t \in [0, 1]$ is a non-dimensional loading parameter. Fig. 1a shows the stress-displacement curve obtained

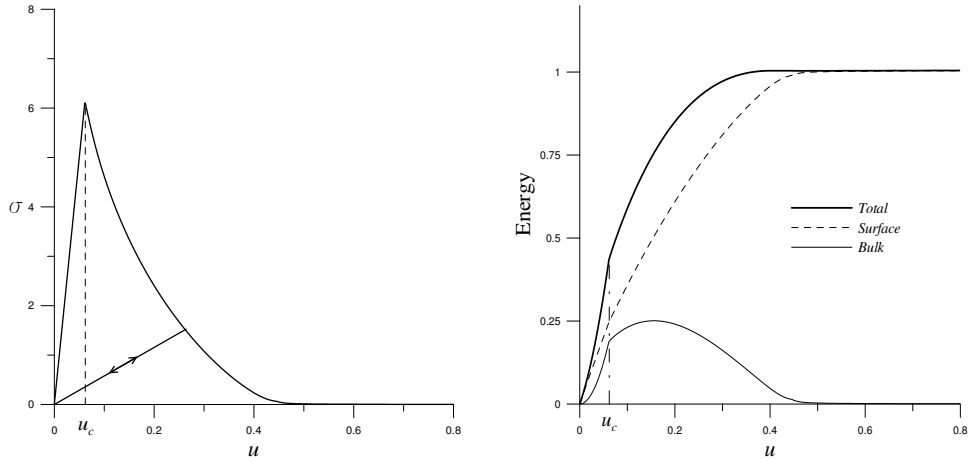


Figure 1: Bar in traction: a) Stress as a function of the imposed displacement; b) total energy as a function of the displacement: bulk contribution and surface contribution.

from FEM calculation. We observe two main phases of the cohesive fracture formation: non-fractured up to $u = u_c$ with a nearly uniform degradation along the bar, and damaged (pre-fractured) for $u > u_c$ up to complete decohesion in which strain and damage clearly localize in some portion of the bar. In this phase cohesive forces appear and vanish as the deformation increases. The unloading-reloading path is also outlined, it follows a linear path. Complete fracture in the sense of Griffith's model can be achieved as $u \to \infty$.
We also investigate the energetic evolution in Fig. 1b, where the total energy, as well as its bulk and surface contributions, are plotted as functions of the displacement. Note that in the displacement interval $[0, u_c]$ evolution follows the elastic deformation: the bulk contribution moves from convex to concave behavior. Moreover, note that the truncation in (3) allows to obtain a bulk contribution which is quadratic near the origin. The total energy together with the surface contribution grow asymptotically up to the value γ, meanwhile the bulk counterpart vanishes. Even, the total energy moves from convex to concave evolution for $u = u_c$.

References

[1] Ambrosio, L., Tortorelli, V.M. 1990, *Approximation of functionals depending on jumps by elliptic functionals via* Γ*-convergence* Comm. Pure Appl. Math., 3, 999-1036.

[2] Ambrosio, L., Tortorelli, V. M. 1992 *On the approximation of free discontinuity problems*, Boll. Un. Mat. Ital. B 7, 105-123.

[3] Barenblatt, G. I. 1962 *The mathematical theory of equilibrium cracks in brittle fracture* Advances in Applied Mechanics. 7, 55–129.

[4] Francfort, G. A. and Marigo, J. J. 1998, *Revisiting brittle fracture as an energy minimization problem*, J. Mech. Phys. Solids, 46, 1319-1342.

[5] Bourdin, B., Francfort, G. A. and Marigo, J. J. 2000, *Numerical experiments in revisited brittle fracture*, J. Mech. Phys. Solids, 48, 797-826.

[6] Bourdin, B., Francfort, G. A., and Marigo, J.-J. 2008, *The variational approach to fracture*, J. Elasticity, 91, 5-148.

[7] Conti, S., Focardi, M., and Iurlano, F. 2015 *Phase field approximation of cohesive fracture models*, Ann. Inst. H. Poincare Anal. Non Lineaire .

[8] Dal Maso, G., Zanini, C. 2007 *Quasi-static crack growth for a cohesive zone model with prescribed crack path*, Proc. Roy. Soc. Edinburgh Sect. A, 137 , 253- 279.

[9] Freddi, F., Iurlano, G., 2016 *Numerical validation of a smeared approach to variational cohesive fracture*, submitted ot Journal of the Mechanics and Physics of Solids.

[10] Freddi, F., Royer-Carfagni, G., 2010 *Regularized variational theories of fracture: A unified approach*, Journal of the Mechanics and Physics of Solids, 58, 1154-1174.

On the identification of viscoelastic material behavior

Andrei Constantinescu
CNRS - Ecole Polytechnique - Université Paris-Saclay
91128 Palaiseau, France
constant@lms.polytechnique.fr

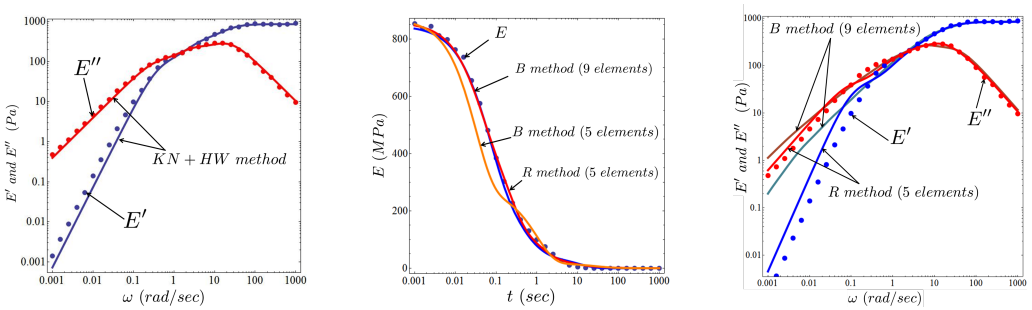
Chiara Daraio
Department of Mechanical and Process Engineering (D-MAVT), Swiss Federal Institute of Technology (ETH)
8092 Zurich, Switzerland
skroedel@ethz.ch

Dimitri Jalocha
Herakles-Safran
dimitri.jalocha@herakles.com

Sebastian Krödel
Department of Mechanical and Process Engineering (D-MAVT), Swiss Federal Institute of Technology (ETH)
8092 Zurich, Switzerland
daraio@ethz.ch

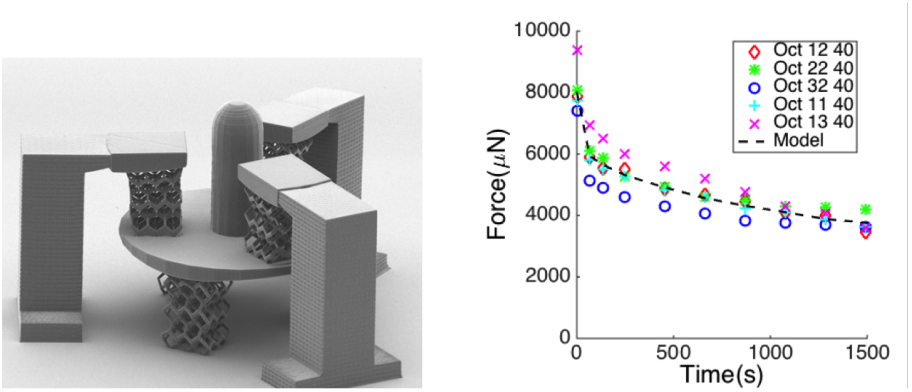
A large class of materials exhibit a viscoelastic behavior. We encounter both natural materials like rubber and various forms of polymers with a homogeneous microstructure and manufactured one like composite, filled polymers where a heterogeneous microstructure has been created. The microstructure plays a key role in the macroscopic mechanical properties of the material. Recently 3D printing or lithographic techniques permit to design micro-architectures materials with specific properties.
The objective of this paper is twofold: (i) to review a series of recent results on the identification of viscoelastic properties [13] and (ii) to explore their application to the identification of viscoelastic parameters for highly filled elastomeric composites and discussing the influence of prestrain [11, 12, 18, 19] and microtruss structures.
The viscoelastic mechanical behavior of the material will be represented using a Generalized Maxwell model [6] and its parameters will be identified from *relaxation* or *Dynamical Mechanical Analysis* (DMA) experiments.
The identification of the relaxation spectrum of a viscoelastic system, corresponds to the determination of the relaxation kernel in an integral equation and is denoted as a Fredholm integral equation of the first kind. The problem has attracted a lot of attentions during the last decades due to its inherent difficulties. It is mathematically ill-posed, implying that the identification of the kernel is not uniquely assured and that small errors in the initial data will conduct to high discrepancies in the identified kernel. Within the recent mathematical literature, we can cite the work of Grasselli [8], Janno et al [14], Von Wolfersdorf [20], Cavaterra et al [4], which recovered the relaxation spectrum by

reducing the problem to a nonlinear Volterra integral equation using a Fourier method to solve the direct problem and by applying the contraction principle. Further results reveled that the problem can also be solved in a heterogeneous medium, as in Lorenzi [16], Lorenzi and Romanov [17] or recently de Buhan and Osses [2] meaning that a spatial material heterogeneity can also be recovered if specific conditions are satisfied. In



(a) (b) (c)

Figure 1: Comparison for the complex modulus of the perturbed data with 5% noise (points) with the identified generalized Maxwell model (continuous line): on panel (a) *KN+HW method* with 3 elements (KN relaxation times),(b) Relaxation modulus data, with the predicted generalized Maxwell model given by the B method and the R method. (c) Complex modulus data, with the predicted complex modulus given by "B method" and "R method".



(a) (b)

Figure 2: (a) The specimen based on microtruss with an octahedron cell used for the relaxations and DMA measurements. (b) A typical relaxation curve for the microtruss structure.

order to eliminate the ill-posedness of the identification problem, a standard technique consists of defining *a priori* the characteristic times for the Prony's series and pursuing the identification only for the elastic moduli of the different elements. This technique is described for example in [9, 10] for the DMA experiments, where the identification is performed on the complex moduli of the material. A recent application example is given in [5], where a generalized Maxwell model is identified to describe the viscoelastic behavior of shape memory polymers. For the relaxation experiment a dual method is proposed in [1, 7] where the relaxation modulus is identified. Other techniques are based

on different numerical schemes to tackle this problem, as for example the combination of Laplace transform and Padé approximants reported in [3], or the cumulative relaxation spectrum proposed in [21].
The improvements of the existing techniques address the distributions of characteristic times. In the case of a DMA experiment, the improvement is based on a mathematical result given by Krein and Nudelmann [15], which permits to identify the relaxation times as the zeros of two complex functions constructed from the measured data [13].
This problem setting does not eliminate the ill-posedness of the initial problem. Two algorithmic matrices have to be positive definite in order to numerically solve the problem and this is realized through a regularization technique. However this imposes more natural restrictions in the problem when compared with an artificial set of characteristic times.In the case of the relaxation experiments, the idea is to optimize the *a priori* set of relaxation time by imposing a closer representation of the relaxation function by reanalyzing the Riemann integration process.
Results for both relaxation and DMA experiments provide a smaller number of branches in the generalized Maxwell model than traditional methods and keep the quality of the representation (see figure 1).

Acknowlegment Different parts of this project have benefited from financing through several programs: French Direction Generale de l'Armement, Laurent Munier (DGA) and HERAKLES-SAFRAN for the PhD of DJ and ANR-15-CE29-0024, DGA-ERE-2015926 and SNF-164375 for the microtruss experiments.

References

[1] M. Baumgaertel and H. Winter. Interrelation between continuous and discrete relaxation time spectra. *Journal of Non-Newtonian Fluid Mechanics*, 44:15–36, 1992.

[2] M. Buhan and A. Osses. Logarithmic stability in determination of a 3d viscoelastic coefficient and a numerical example. *Inverse Problems*, 26:1088–1112, 2010.

[3] C. Carrot and V. Verney. Determination of discrete relaxation spectrum from dynamic experimental data using the pade laplace method. *European Polymer Journal*, 32:69–77, 1996.

[4] C. Cavaterra and M. Grasselli. On an inverse problem for a model of linear viscoelastic Kirchhoff plate. *Journal of Integral Equation Applied*, 9:179–218, 1997.

[5] J. Diani and P. Gilormini and C. Fredy and I. Rousseau Predicting thermal shape memory of crosslinked polymer networks from linear viscoelasticity *International Journal of Solids and Structures*, 49:793–799, 2012.

[6] W. Findley, J. Lai, and K. Onaran. *Creep and Relaxation of Nonlinear Viscoelastic Materials*. 1976.

[7] S. Gerlach and A. Matzenmiller. Comparison of numericla methods for identification of viscoelastic line spectra from static test data. *International Journal for Numerical Methods in Engineering*, 63:428–454, 2005.

[8] M. Grasselli. Determining the relaxation tensor in linear viscoelasticity of integral type. *Japan Journal of Industrial and Applied Mathematics*, 11:13153, 1994.

[9] J. Honerkamp. Ill-posed problems in rheology. *Rheologica Acta*, 28:363–371, 1989.

[10] J. Honerkamp and J. Weese. Tikhonovs regularization method for ill-posed problems. *Continuum Mechanics and Thermodynamics*, 2:1730., 1990.

[11] Jalocha, D., Constantinescu, A., and Neviere, R. Prestrained biaxial dma investigation of viscoelastic nonlinearities in highly filled elastomers. *Polymer Testing*, 42:37–44, 2015. dx.doi.org/10.1016/j.polymertesting.2015.01.005.

[12] Jalocha, D., Constantinescu, A., and Neviere, R. Pre–strain dependent viscosity of highly filled elastomer: Experiments and modeling. *Mechanics of Time-Dependent Materials*, 2015. dx.doi.org/10.1007/s11043-015-9262-z.

[13] Jalocha, D., Constantinescu, A., and Neviere, R. Revisiting the identification of generalized maxwell models from experimental results. *International Journal of Solids and Strucures*, 2015. dx.doi.org/10.1016/j.ijsolstr.2015.04.018.

[14] J. Janno and L. Von Wolfersdorf. Inverse problems for identification of memory kernels in viscoelasticity. *Mathematical Methods for Applied Science*, 20:291–314, 1997.

[15] M Krein and A Nudelman. An interpolation problem in the class of stieltjes functions and its connection with other problems. *Integral Equations and Operator Theory*, 30:251–278, 1998.

[16] A. Lorenzi. A multidimensional identification problem related to a hyperbolic integrodifferential equation. *Zeitschrift fur Analysis und ihre Anwendungen*, 18:407–435, 1999.

[17] A. Lorenzi and V. Romanov. Stability estimates for an inverse problem related to viscoelastic media. *Journal of Inverse Ill-Posed Problems*, 18:407–435, 2006.

[18] Thorin, A., Azoug, A., and Constantinescu, A. Influence of prestrain on mechanical properties of highly-filled elastomers: Measurements and modeling. *Polymer Testing*, 31:978–986, 2013. dx.doi.org/10.1016/j.polymertesting.2012.07.014.

[19] Thorin, A., Azoug, A., Neviere, R., Constantinescu, A., and Praidelles-Duval. Influence of orthogonal prestrain on the viscoelastic properties of highly-filled elastomers: Measurements and modeling. *Polymer Testing*, 32:8, 2013. dx.doi.org/10.1016/j.polymertesting.2012.12.005.

[20] L. Von Wolfersdorf. On identification of memory kernels in linear viscoelasticity. *Mathematische Nachriten*, 161:203–217, 1993.

[21] R. Xiao and J. Choi and N. Lakhera and C. Yakacki and C. Frick and T. Nguyen Modeling the glass transition of amorphous networks for shape memory behavior. *Journal of the Mechanics and Physics of Solids*, 61:1612–1635, 2013.

[22] M. Zarrelli and .A. Skordos and.K. Partridge. Toward a constitutive model for cure-dependent modulus of a high temperature epoxy during the cure. *European Polymer Journal*, 46:1705–1712, 46.

Passing from Adhesive Contact to Brittle Delamination in Visco-Elastodynamics

Riccarda Rossi
DIMI – Università degli Studi di Brescia
via Branze, 38 25133 - Brescia Italy
riccarda.rossi@unibs.it

Marita Thomas
Weierstrass Institute for Applied Analysis and Stochastics
Mohrenstr., 39 10117 - Berlin Germany
marita.thomas@wias-berlin.de

Adhesive contact between two elastic bodies along a prescribed surface can be modeled in terms of an adhesive parameter (accounting for the proportion of active bonds between the bodies), governed by a rate-independent flow rule which is coupled to the momentum balance with viscosity and inertia.
Through a rigorous asymptotics, we investigate the relation of this model to a model brittle delamination, extending previous results in [1, 2]. In the brittle case, the momentum balance and the flow rule for the adhesion parameter are coupled via a constraint on the contact surface imposing a transmission condition on the displacements on the set where the bonding is active, and allowing for jumps on the crack set, and this system can be thus understood as a model of dynamic fracture (along a prescribed surface).

References

[1] Roubíček, T. and Scardia, L. and Zanini, C. 2009 *Quasistatic delamination problem.* Continuum Mech. Ther-modynam. 21, 223–235.

[2] Rossi, R. and Thomas, M. 2015 *From an adhesive to a brittle delamination model in thermo-visco-elasticity.* ESAIM Control Optim. Calc. Var. 21,1–59.

A two-scale criterion to predict high-cycle fatigue crack initiation in shape memory alloys

Giulia Scalet
Università di Pavia
via Ferrata, 1 27100 - Pavia Italy
giulia.scalet@unipv.it

Ferdinando Auricchio
Università di Pavia
via Ferrata, 1 27100 - Pavia Italy
auricchio@unipv.it

Andrei Constantinescu
Ecole Polytechnique, CNRS, Université Paris-Saclay
Route de Saclay, 91128 - Palaiseau France
constant@lms.polytechnique.fr

Costantino Menna
Università di Napoli 'Federico II'
via Claudio, 21 80125 - Napoli Italy
costantino.menna@unina.it

Shape memory alloys (SMAs) are smart materials which possess unique properties, known as shape memory effect and pseudo-elasticity. Such properties result from reversible diffusionless solid-solid transformations between a parent and a product phase, called, respectively, austenite and martensite.
SMA devices are often subjected to thousand or millions of in-service loading cycles and thus fatigue failure represents an important design issue, which limits component lifetime. A typical example is given by cardiovascular stents which are subjected to pulsatile loading. The prediction of crack initiation and growth is an essential design requirement and necessitates a thorough understanding of the effect of microstructural phase evolution on fatigue damage. Particularly, to achieve high durability requirements in the design process, there is a special interest in the high-cycle fatigue (HCF) regime, where energy dissipation remains bounded in time. From the theoretical viewpoint, classical fatigue methodologies for infinite and finite lifetime cannot be directly employed, due to the unusual fatigue behavior of SMAs [5].
This work proposes a fatigue methodology to predict infinite lifetime in polycrystalline SMAs. According to physical observations showing that fatigue damage is controlled by mechanisms at the grain scale in a polycrystalline material, we study the HCF problem through the introduction of the mesoscopic grain scale, in addition to the macroscopic scale of continuum mechanics. The analysis is based on recent mathematical advancements on shakedown theorems [2] and on the rigorous framework of standard generalized materials. A fatigue criterion of the Dang Van-type [1] is then proposed; it (i) is based on a two-scale approach considering both austenite and martensite (see Figure 1), (ii) is multiaxial, and

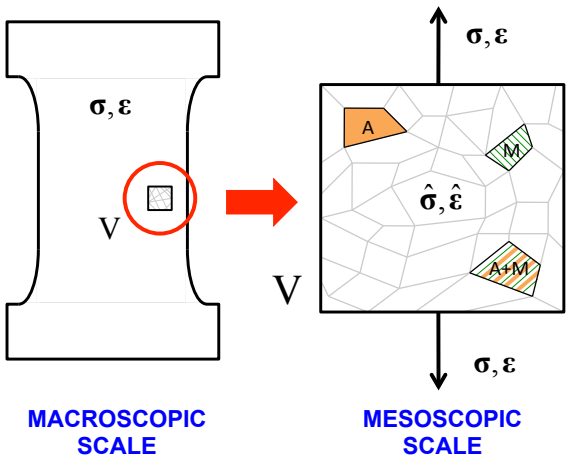


Figure 1: Schematic representation of the macroscopic scale of a SMA body and the mesoscopic scale of the representative volume V. The volume consists of austenite (A), martensite (M), and mixed martensite and austenite (A + M) grains. Mesoscopic and macroscopic quantities are denoted with and without an hat, respectively (i.e., stresses $\boldsymbol{\sigma}$ and $\hat{\boldsymbol{\sigma}}$ and strains $\boldsymbol{\varepsilon}$ and $\hat{\boldsymbol{\varepsilon}}$).

(iii) predicts HCF crack initiation. The multiscale approach is settled on the assumption that, under HCF, a fatigue crack will not initiate if an elastic shakedown state is reached at both macroscopic and mesoscopic scale. In other words, if the following condition:

$$\max_{t>t_0}\{\hat{\tau}(\mathbf{x},t) + a(\boldsymbol{\alpha}(\mathbf{x}))\hat{\sigma}_h(\mathbf{x},t)\} \leq b(\boldsymbol{\alpha}(\mathbf{x})) \tag{1}$$

is not satisfied in all the points $\mathbf{x}$ of the structure at any time t, a fatigue crack will initiate and the structure will have a finite lifetime. In condition (1), $\hat{\tau}$ and $\hat{\sigma}_h$ are the mesoscopic shear stress and hydrostatic stress, respectively; the variable $\boldsymbol{\alpha}$ represents the inelastic strain and can include the description of several physical phenomena characterizing SMA behavior, e.g., permanent plasticity, phase transformations, or void generation and fracture; a and b are material parameters depending on $\boldsymbol{\alpha}$. For the simulations, the well-known three-dimensional constitutive Souza-Auricchio model for SMAs is employed [4], where $\boldsymbol{\alpha}$ denotes the transformation strain tensor. The criterion is calibrated and validated on experiments from the literature [3]. The application to a cardiovascular stent is also presented. Several loading conditions are considered, together with the interaction between stent, vessel, and plaque. The effect of the martensite volume fraction distribution on stent fatigue is investigated (see Figure 2).
The results permit a novel insight into the analysis of the onset of damage in materials involving phase change and raise novel questions on microscopic deformation, damage mechanisms at phase boundaries, and experimental methods for the identification of fatigue limits.

References

[1] Dang Van, K. 1999. High-cycle metal fatigue in the context of mechanical design. In *CISM Courses and Lectures* (ed. K. Dang Van and I. Papadopoulos). no 392, pp. 57–88. Springer.

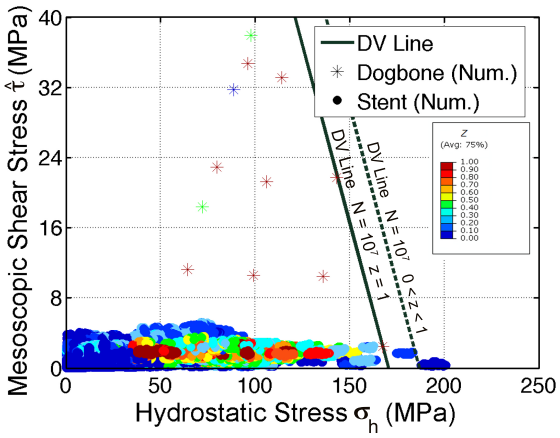


Figure 2: Application of the proposed criterion of the Dang Van (DV) type to the stent. The results are reported in the DV fatigue diagram in terms of mesoscopic shear stress and hydrostatic stress. Each point is characterized by a value of the martensite volume fraction z. The experimental results on dogbones provided in [3] are also reported.

[2] Peigney, M. 2014 *On shakedown of shape memory alloys structures.* Ann. Solid Struct. Mech. 6 (1-2), 17–28.

[3] Pelton, A. 2011 *Nitinol Fatigue: A Review of Microstructures and Mechanisms.* J. Mater. Eng. Perform. 20 (4-5), 613–617.

[4] Souza, A., Mamiya, E., Zouain, N. 1998 *Three-dimensional model for solids undergoing stress-induced phase transformations.* Eur. J. Mech. A-Solid 17, 789–806.

[5] Robertson, S., Pelton, A., and Ritchie, R. 2012 *Mechanical fatigue and fracture of Nitinol.* Int. Mater. Rev. 57 (1), 1–37.

Modeling Dissipative Phenomena - Part II: Diffuse interface models

PROPOSERS

Maurizio Grasselli
Politecnico di Milano
P.zza Leonardo da Vinci, 32 20133 - Milano - Italy
maurizio.grasselli@polimi.it

Elena Bonetti
Università degli Studi di Milano

Cecilia Cavaterra
Università degli Studi di Milano

Monica Conti
Politecnico di Milano

SPEAKERS

Stefania Gatti
Università degli Studi di Modena e Reggio Emilia
stefania.gatti@unimore.it

Andrea Giorgini
Politecnico di Milano
andrea.giorgini@polimi.it

Alain Miranville
Université de Poitiers
alain.miranville@math.univ-poitiers.fr

Elisabetta Rocca
Università degli Studi di Pavia
elisabetta.rocca@unipv.it

Sergio Frigeri
WIAS, Berlin
frigeri@wias-berlin.de

Jürgen Sprekels
WIAS, Berlino
jurgen.sprekels@wias-berlin.de

Dissipation of energy is ubiquitous in Nature. Damage, viscoelasticity, phase changes are just some important examples of such phenomena. They are all characterized by an energy which decreases over time. The goal of this minisymposium is to present an up-to-date overview of their mathematical treatment. The minisymposium is divided into two parts. The first is devoted to mathematical models of damaging, fatigue, aging

and viscoelasticity. All these phenomena are related to a losing of elastic response of materials, which may decrease in time or due to the damaging of internal cohesion bonds. The second is concerned with diffuse interface models which have recently received a lot of attention since they can be employed to describe a large variety of phenomena. In particular, we recall phase separation, tumor growth, image inpainting and liquid crystals.

Multi-component Cahn-Hilliard systems with dynamic boundary conditions

Stefania Gatti
Università degli Studi di Modena e Reggio Emilia
Dipartimento FIM, via Campi 213/B, 41125 - Modena Italy
stefania.gatti@unimore.it

Monica Conti
Politecnico di Milano
Dipartimento di Matematica "F. Brioschi"
Via Bonardi 9, 20133 Milano, Italy
monica.conti@polimi.it

Alain Miranville
Université de Poitiers
Laboratoire de Mathématiques et Applications, UMR CNRS 7348 - SP2MI
Boulevard Marie et Pierre Curie - Téléport 2
86962 Chasseneuil Futuroscope Cedex, France
Alain.Miranville@math.univ-poitiers.fr

This talk is concerned with the well-posedness and the asymptotic behavior, in terms of finite-dimensional attractors, of Cahn-Hilliard systems describing phase separation processes in multi-component alloys, endowed with dynamic boundary conditions. Such boundary conditions take into account the interactions with the walls when considering confined systems.

The nonlocal Cahn-Hilliard equation with singular potential: separation property and regularity results

Andrea Giorgini
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
andrea.giorgini@polimi.it

Ciprian G. Gal
Florida International University
11200 S.W. 8th Street - Miami, Florida
cgal@fiu.edu

Maurizio Grasselli
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
maurizio.grasselli@polimi.it

In Material Science the Cahn-Hilliard system has been introduced in [1] to describe at a macroscopic level the formation and evolution of microstructures during the phase segregation in a binary alloys system. This phenomenon occurs when a homogeneous mixture undergoes a rapid cooling below a critical temperature. More recently, a nonlocal version of the Cahn-Hilliard system has been proposed in [2] and [3]. This macroscopic equation has been rigorously derived starting from a microscopic formulation and taking into account long range repulsive interactions between different species and short hard collisions between all particles. The resulting model is the conserved gradient flow associated to the nonlocal Helmholtz free energy

$$\mathcal{E}(\varphi) = -\frac{1}{2}\int_\Omega\int_\Omega J(x-y)\varphi(x)\varphi(y)\,dx\,dy + \int_\Omega F(\varphi)\,dx$$

and reads as

$$\begin{cases} \varphi_t = \Delta\mu, \\ \mu = F'(\varphi) - J*\varphi, \end{cases} \qquad \text{in } \Omega\times(0,T).$$

Here Ω is a bounded domain $\mathbb{R}^d$, $d=2,3$, φ is the relative difference of the two concentrations, μ is the chemical potential, θ is the absolute temperature and F is the physically relevant potential defined by

$$F(s) = \frac{\theta}{2}\left[(1+s)\log(1+s) + (1-s)\log(1-s)\right], \quad \forall\, s\in(-1,1).$$

The aim of this talk is to discuss some recent results on the longtime regularity of weak solutions and the validity of the separation property.

References

[1] J.W. Cahn and J.E. Hilliard, Free energy of a nonuniform system. I. Interfacial free energy, J. Chem. Phys. 28 (1958), 258-267.

[2] G. Giacomin and J.L. Lebowitz, Phase segregation dynamics in particle systems with long range interactions. I. Macroscopic limits, J. Statist. Phys. 87 (1997), 37-61.

[3] G. Giacomin and J.L. Lebowitz, Phase segregation dynamics in particle systems with long range interactions. II. Interface motion, SIAM J. Appl. Math. 58 (1998), 1707-1729.

Cahn-Hilliard inpainting

Alain Miranville
Université de Poitiers
Mathématiques, SP2MI, 86962 Chasseneuil Futuroscope Cedex
miranv@math.univ-poitiers.fr

Our aim in this talk is to discuss variants of the Cahn-Hilliard equation in view of applications to image inpainting. We will present theoretical results as well as numerical simulations.

Diffuse and sharp interfaces in Biology and Mechanics

Elisabetta Rocca
Università degli Studi di Pavia
via Ferrata, 1 27100 - Pavia Italy
elisabetta.rocca@unipv.it

In this contribution we present the idea of joining different real-world applications coming from Biology and Fluid Mechanics under the common feature of diffuse interface problems and of the need of a suitable weak solution notion for the corresponding PDE systems. The following fields of interest are indeed particularly challenging nowadays: tumor growth models, damage in elasto-plastic materials, two-fluids flows and liquid crystal dynamics. The main focus of this presentation regards recent modelling and analysis of tumor growth dynamics. This has indeed recently become a major issue in applied mathematics (see, e.g., [4] and references therein). In this new approach sharp interfaces are replaced by narrow transition layers arising due to adhesive forces among the cell species. Hence, a continuum thermodynamically consistent model is introduced. However, while numerical simulations of diffuse-interface type models for tumor growth have been carried out in several papers (cf., e.g., Chap.8 in [4]), nonetheless, a rigorous mathematical analysis of the resulting systems of PDEs is still in its infancy.
In the very recent papers [2], [3], and [6], we consider a diffuse interface model for tumor growth proposed [7]. This model consists of the Cahn-Hilliard equation for the tumor cell fraction nonlinearly coupled with a reaction-diusion equation for the nutrient-rich extracellular water volume fraction. We shall first present a result on the existence of a weak solution, then we show that the weak solution is unique and continuously depends on the initial data. Furthermore, we shall give a result on the existence of a strong solution that allows to show that any weak solution regularizes in nite time. The last results will be on the existence of the global attractor in a phase space characterized by an a priori bounded energy and on some rigorous asymptotics.
However, for instance, one may include the fluid velocity either given as a datum or satisfying a generalized Darcy's (or Brinkman's) law. In this spirit we aim to report on the recent paper [5] where we consider a diffuse interface model for tumor growth recently proposed in [1]. The resulting PDE system couples four different types of equations: a Cahn-Hilliard type equation for the tumor cells (which include proliferating and dead cells), a Darcy law for the tissue velocity field, whose divergence may be different from 0 and depend on the other variables, a transport equation for the proliferating (viable) tumor cells, and a quasi-static reaction diffusion equation for the nutrient concentration. We establish existence of weak solutions for the PDE system coupled with suitable initial and boundary conditions. In particular, the proliferation function at the boundary is supposed to be nonnegative on the set where the velocity $\mathbf{u}$ satisfies $\mathbf{u} \cdot \nu > 0$, where ν is the outer normal to the boundary of the domain. We also study a singular limit as the diffuse interface coefficient tends to zero in order to pass from diffuse to sharp interfaces. Finally, we will leave some space to introduce other diffuse interface models in (Fluid)

Mechanics (damage, two-phase fluids, liquid crystals), which can be treated with similar techniques.

References

[1] Y. Chen, S.M. Wise, V.B. Shenoy, J.S. Lowengrub, *A stable scheme for a nonlinear, multiphase tumor growth model with an elastic membrane*, Int. J. Numer. Methods Biomed. Eng. **30** (2014), 726–754.

[2] P. Colli, G. Gilardi, E. Rocca, J. Sprekels, *Vanishing viscosities and error estimate for a Cahn–Hilliard type phase field system related to tumor growth*, Nonlinear Analysis: Real World Applications, **26** (2015), 93–108.

[3] P. Colli, G. Gilardi, E. Rocca, J. Sprekels, *Asymptotic analyses and error estimates for a Cahn–Hilliard type phase field system modelling tumor growth*, preprint arXiv:1503.00927v1 (2015), 1–19, DCDS-S issue from the STAMM in Poitiers, to appear (2015).

[4] V. Cristini, J. Lowengrub, *Multiscale modeling of cancer. An Integrated Experimental and Mathematical Modeling Approach*, Cambridge Univ. Press, 2010.

[5] M. Dai, E. Feireisl, E. Rocca, G. Schimperna, M. Schonbek, *Analysis of a diffuse interface model of multispecies tumor growth*, preprint arXiv:1507.07683 (2015), 1–18, WIAS preprint No. 2150 (2015), 1–22.

[6] S. Frigeri, M. Grasselli, E. Rocca, *On a diffuse interface model of tumor growth*, European J. Appl. Math. 26 (2015).

[7] A. Hawkins-Daarud, K.G. van der Zee, J.T. Oden, *Numerical simulation of a thermodynamically consistent four-species tumor growth model*, Int. J. Numer. Meth. Biomed. Engng. **28** (2011), 3–24.

On some nonlocal diffuse-interface models for binary fluids: regularity results and applications

Sergio Frigeri
Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Berlin,
Mohrenstrasse 39, 10117, Berlin.
frigeri@wias-berlin.de

We shall first review the basic features and mathematical results concerning models for flow and phase separation of mixtures of viscous incompressible fluids, which are based on nonlocal Cahn-Hilliard/Navier-Stokes systems. The nonlocal Cahn-Hilliard/Navier-Stokes (CHNS) system has been studied analytically in a series of papers (cf. [1, 4, 5, 6, 7, 3, 8] and, more recently, [2]). We shall then present the more recent results, under different assumptions on the double-well potentials, mobility and viscosity of the two fluids of the mixture. These will concern, in particular, existence of strong solutions in two dimensions. We shall also focus our attention on the physically relevant and mathematically challenging situation where the viscosity depends on the order parameter. Finally, we shall talk about the main applications of these results to some important topics, namely, to optimal control and long time behavior analysis. The presented recent results are obtained jointly with C. Gal, M. Grasselli and J. Sprekels.

References

[1] P. Colli, S. Frigeri and M. Grasselli, *Global existence of weak solutions to a nonlocal Cahn-Hilliard-Navier-Stokes system*, J. Math. Anal. Appl. **386** (2012), 428-444.

[2] S. Frigeri, *Global existence of weak solutions for a nonlocal model for two-phase flows of incompressible fluids with unmatched densities*, WIAS Preprint **2117** (2015).

[3] S. Frigeri, C. Gal and M. Grasselli, *On nonlocal Cahn-Hilliard-Navier-Stokes systems in two dimensions*, to appear on J. Nonlinear Sci., DOI 10.1007/s00332-016-9292-y.

[4] S. Frigeri and M. Grasselli, *Global and trajectory attractors for a nonlocal Cahn-Hilliard-Navier-Stokes system*, J. Dynam Differential Equations **24** (2012), 827-856.

[5] S. Frigeri and M. Grasselli, *Nonlocal Cahn-Hilliard-Navier-Stokes sy-stems with singular potentials*, Dyn. Partial Differ. Equ. **9** (2012), 273-304.

[6] S. Frigeri, M. Grasselli and P. Krejčí, *Strong solutions for two-dimensio-nal nonlocal Cahn-Hilliard-Navier-Stokes systems*, J. Differential Equations **255** (2013), 2587-2614.

[7] S. Frigeri, M. Grasselli and E. Rocca, *A diffuse interface model for two-phase incompressible flows with nonlocal interactions and nonconstant mobility*, Nonlinearity **28** (2015), 1257-1293.

[8] S. Frigeri, E. Rocca and J. Sprekels, *Optimal distributed control of a nonlocal Cahn–Hilliard/Navier–Stokes system in 2D*, SIAM J. Control Optim. **54** (2016), 221-250.

On a nonstandard viscous Cahn–Hilliard system: existence and optimal control

Jürgen Sprekels
WIAS
10117 Berlin, Germany
juergen.sprekels@wias-berlin.de

Pierluigi Colli
Università di Pavia
Via Ferrata 1, 27100 Pavia, Italy
pierluigi.colli@unipv.it

Gianni Gilardi
Università di Pavia
Via Ferrata 1, 27100 Pavia, Italy
gianni.gilardi@unipv.it

We study nonstandard viscous Cahn–Hilliard type system that was introduced by P. Podio-Guidugli as a model for dissipative phase separation. It consists of a system of two partial differential equation for the two unknown functions, which are given by the chemical potential and the order parameter of the phase transition process. The PDE system is highly nonlinear, exhibiting unpleasant nonlinear couplings involving the time derivatives of the unknowns that render the analysis difficult. In this talk, recent results concerning well-posedness, stability, regularity, and optimal control problems associated with the phase separation process will be discussed.

Advances in Quantitative Finance - Part I: recent perspectives

PROPOSERS

Chiara Guardasoni
Dip. di Matematica e Informatica, Università degli Studi di Parma
Parco Area delle Scienze, 53/A 43124 - Parma Italy
chiara.guardasoni@unipr.it

Daniele Marazzina
Dip. di Matematica, Politecnico di Milano
Via Bonardi, 9 20133 - Milano Italy
daniele.marazzina@polimi.it

Simona Sanfelici
Dip. di Economia, Università degli Studi di Parma
Via Kennedy, 6 43125 - Parma Italy
simona.sanfelici@unipr.it

SPEAKERS

Giorgia Callegaro
Dip di Matematica, Università degli Studi di Padova
gcallega@math.unipd.it

Lorella Fatone
Scuola di Scienze e Tecnologie, Università di Camerino
lorella.fatone@unicam.it

Gianluca Fusai
Dip. di Scienze Economiche e Metodi Quantitativi, Università degli Studi del Piemonte Orientale
gianluca.fusai@eco.unipmn.it

Emanuele Nastasi
Dip. di Matematica, Politecnico di Milano
emanuele.nastasi@polimi.it

Fabio Della Marra
Dip. di Economia, Università degli Studi di Parma
fabio.dellamarra@studenti.unipr.it

Marianito Rodrigo
Dept. of Engineering and Information Sciences, University of Wollongong (Australia)
marianit@uow.edu.au

In recent years the research for mathematical tools to be applied in financial contexts has gained additional importance. In fact the latest financial crisis has highlighted the need for a more scientific approach to the problem of pricing and risk control. Moreover,

we can now take advantage of more advanced statistical and mathematical skills and of the availability of numerical techniques and faster computer systems.

In this minisymposium, a variety of advanced mathematical modelling tools, numerical methods and scientific computation techniques for different current problems in quantitative finance will be presented. More precisely, this first part of the minisymposium is devoted to present recent contributions of applied mathematics in solving financial problems.

Vector quantization: recent perspectives

Giorgia Callegaro
Università degli Studi di Padova
via Trieste, 63 35121 - Padova Italy
gcallega@math.unipd.it

The birth of optimal quantization dates back to the 50's, when the necessity to optimize signal transmission by appropriate discretization procedures arose. Quantization consists in approximating a signal admitting a continuum of possible values, by a signal that takes values in a discrete set. *Vector quantization* deals with signals that are finite dimensional, such as random variables, while *functional quantization* extends the concepts to the infinite-dimensional setting, as it is the case of stochastic processes. Quantization of random vectors can be considered as a discretization of the probability space, providing the "best" approximation to the original distribution. It is therefore crucia to optimize the geometric location of these "points" and to evaluate the resulting error. Some numerical procedures have been developed in order to get optimal quadratic quantization of the most known distributions (e.g. the Gaussian) in high dimension, mostly based on stochastic optimization algorithms. Over the years many other application fields have been discovered and this opened the door to new research perspectives in Numerical Probability and applications to Mathematical Finance. For a comprehensive introduction to optimal vector quantization and its applications, we refer to [2] and references therein.

While theoretically sound and deeply investigated, optimal quantization typically suffers from the numerical burden that the algorithms involve. The main reason is related to the highly time-consuming procedure required by the determination of the optimal grid, especially in the multi-dimensional case where stochastic algorithms are necessary. Recently a very promising type of quantization, called *recursive marginal quantization*, has been introduced by [3] and it has been tested in a pricing context. This new approach provides sub-optimal quantization grids in a very accurate and fast way, so that it has been possible to use it for the first time to deal with market data, in a calibration perspective and to price non-vanilla derivatives in diffusive market models (see [1]).

The aim of the talk is illustrating the most recent research in vector quantization applied to numerical probability, by presenting newly discovered efficient discretization algorithms and their applications to mathematical finance. Open questions and possible research directions to follow will hopefully foster discussion with the audience.

References

[1] Callegaro, G., Fiorin, L. and Grasselli, M. 2015 *Quantized calibration in local volatility.* Risk Magazine 28(4) , 62–67.

[2] Graf, S. and Luschgy, H. 2000 Foundations of quantization for probability distributions. Springer, New York.

[3] Pages, G. and Sagna, A. 2015 *Recursive marginal quantization of the Euler scheme of a diffusion process.* Applied Mathematical Finance 22(5), 463–498.

Dynamical models of banking system and systemic risk governance via stochastic optimal control

Lorella Fatone
Università degli Studi di Camerino
Via Madonna delle Carceri 9, 62032 Camerino Italy
lorella.fatone@unicam.it

We consider the problem of governing systemic risk in two banking system models (see [1], [2]). The monetary authority is responsible for the governance of the banking systems. In these models the dynamics of the banking system is defined implicitly by an initial value problem for a system of stochastic differential equations. In the first model the dependent variables of the differential equations are the log-monetary reserves of the banks as functions of time, while in the second model the dependent variables are the assets and the liabilities of the banks as functions of time. The models proposed generalize those presented in [3] and describe homogeneous populations of banks. Distinct mechanisms are used to describe different forms of cooperation between banks and the intervention of the monetary authority in the banking systems. In the models studied a bank fails when its log-monetary reserves or its capital reserves go below an assigned default level. We call systemic risk or systemic event in a bounded time interval the fact that in that time interval at least a given fraction of the banks fails. The probability of systemic risk in a bounded time interval is evaluated using statistical simulation. The goal of the systemic risk governance is to keep the probability of systemic risk in a bounded time interval between two given thresholds. The systemic risk governance consists in the choice of the log-monetary reserves (first model) or of the assets and of the liabilities (second model) of a kind of "ideal bank" as functions of time and in the choice of the rules that regulate the cooperation mechanism among banks. These rules are obtained solving a stochastic optimal control problem for a kind of mean field approximation of the banking system models. A method to govern systemic risk in a bounded time interval is presented and some numerical examples of systemic risk governance of banking systems in presence and in absence of shocks are discussed.

References

[1] Fatone, L., Mariani, F., Recchioni, M.C. and Zirilli, F. 2015 *Systemic risk governance in a dynamical model of a banking system*, submitted.

[2] Fatone, L., Mariani, F., Recchioni, M.C. and Zirilli, F. 2016 *An assets-liabilities dynamical model of a banking system and systemic risk governance*, in preparation.

[3] Fouque, J.-P. and Sun, L. H. 2013 *Systemic risk illustrated*. In *Handbook of Systemic Risk* (ed. J.-P. Fouque, J. Langsam) pp. 444–452. Cambridge University Press, Cambridge, U.K..

Analysis of Calibration Risk for Exotic Options through a Resampling Technique

Gianluca Fusai
Università degli Studi del Piemonte Orientale
via Perrone, 18 28100 - Novara Italy
gianluca.fusai@eco.unipmn.it

Marina Marena
Department of Economics and Statistics, Università di Torino
Corso Unione Sovietica 218bis, 10134 Torino, Italy
marina.marena@unito.it

Marco Materazzi
Financial Analyst at Source
138 Kingsland Road, London E28DY, UK
marco.materazzi@hotmail.com

Substantial losses suffered by financial institutions, due to mispricing of financial derivatives in the last decades, has lead regulators to address model risk. The Basel Committee on Banking Supervision (2009) identifies two types of model risk: the risk associated with possibly incorrect evaluation of complex products and calibration risk which arises from unobservable model parameters. This risk has to be assessed by financial institutions and valuation adjustments should be introduced to account for it. The Federal Reserve (2011) has drawn guidelines for an active management of model risk. Among other things, the document suggests that banks should employ sensitivity analysis in model development and validation to check the impact of small changes in inputs and parameter values on model outputs. The European Banking Authority has set out requirements relating to additional valuation adjustments (AVA) of fair-valued positions to determine prudent values of balance sheets, which should cover valuation model risk, "which arises due to the potential existence of a range of different models or model calibrations, which are used by market participants, and the lack of a firm exit price for the specific product being valued".
Cont (2006) has built a theoretical framework, extended by Gupta et al. (2010), for the quantification of model uncertainty. In the context of exotic option prices, Schoutens et al. (2004) have analyzed model risk, i.e. the risk related to pricing options using a wrong model, in an empirical study. Moreover, even if an appropriate model has been chosen, so that model risk is ruled out, the calibration procedure of option pricing models to market data has a relevant impact on exotic option prices. This involves several risk dimensions. Detlefsen et al. (2007) have studied calibration risk as arising from the use of different loss functions. Guillaume and Schoutens (2012) extend this concept to include the calibration methodology. Gilli and Schumann (2010) have examined the use of different calibration algorithms.
In this paper, we focus on another dimension of calibration risk, which arises from the estimation error of calibrated model parameters and carries over to exotic prices.

We quantify its impact for some popular option pricing models through a parametric bootstrapping technique. From an econometric point of view, the calibration of the parameters of the preferred model to market quantities consists of a non linear least squares regression. Using asymptotic results, we obtain the bootstrap distribution of the exotic derivative prices. This allows us to compute confidence intervals of exotic option prices that contain the same information brought by the original sample, thus quantifying estimation risk.
We provide empirical evidence of calibration risk for exotic options on a time series of EURO STOXX 50 implied volatility surfaces, covering a one year period. It turns out that complex pricing models provide a better fit to liquid market data, but at a cost of higher uncertainty in pricing exotic products, for which estimation risk can be substantial. Furthermore, we perform a sensitivity analysis along the lines proposed in Baucells and Borgonovo (2013). In finance, a standard way of performing a sensitivity analysis is to compute the so-called option Greeks with respect to the model parameters. However, a fatal limitation of this approach is that, due its intrinsic local nature, it does not take into account model non-linearities and presence of correlations among the unknown model inputs parameters. A natural way to take into account this is the probabilistic Sensitivity Analysis in Baucells and Borgonovo (2013) that identifies key sources of uncertainty in the model output with respect to the uncertainty in model parameters. Our boostrap procedure makes viable the sensitivity analysis for option pricing and for quantitative assessment of the model valuation adjustment. This can be of some value for regulators and risk-managers.

References

[1] BIS, 2009. Revisions to the Basel II market risk framework. Basel Committee on Banking Supervision.

[2] Cont, R. (2006). Model uncertainty and its impact on the pricing of derivative instruments. *Mathematical Finance*, Volume 16, Issue 3, pages 519–547.

[3] Detlefsen, K. and Hardle, W.K. (2007). Calibration risk for exotic options. *The Journal of Derivatives*, Vol. 14, No. 4: pp. 47-63.

[4] EBA, 2014. Final draft Regulatory Technical Standards on prudent valuation under Article 105(14) of Regulation (EU) No 575/2013 (Capital Requirements Regulation — CRR).

[5] Federal Reserve Board, 2011. Supervisory Guidance on Model Risk Management. SR Letter, 11-7.

[6] Gilli, M. and Schumann, E. (2010). Calibrating Option Pricing Models with Heuristics. *Working Papers 030, COMISEF*.

[7] Guillaume, F. and Schoutens, W. (2012). Calibration risk: Illustrating the impact of calibration risk under the Heston model. *Review of Derivatives Research*, pag. 1–23.

[8] Gupta, A., Reisinger, C. and Whitley, A. (2010). Model uncertainty and its impact on derivative pricing, in *Rethinking Risk Management and Reporting: Uncertainty, Bayesian Analysis and Expert Judgement*. Risk Books.

Mapping the basket

Emanuele Nastasi
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
emanuele.nastasi@polimi.it

Roberto Baviera
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
roberto.baviera@polimi.it

We present a new algorithm for computing optimal upper and lower bounds to multivariate European options when the underlying is modelled as a multidimensional geometric Brownian motion. We focus on basket options, which are European options written on a linear combination of stocks. This payoff includes also other derivatives such as Asian options or swaptions when the drift and the volatility are deterministic function of time. The problem is financially relevant because pricing and hedging multivariate claims in several dimensions via numerical techniques can be very time consuming. Moreover, despite the assumption of constant volatility is known to be not true, the Black formula is still extremely popular among practitioners and therefore one can be interested in obtaining a multivariate equivalent of this formula.
In [1] a lower bound for a basket option is derived, which is basically the basket of the options written on the assets within the basket with scaled volatilities. In [2] an upper bound (ICUB) which involves an additional numerical integration is derived. These bounds strongly depend on a variable x which lies on a quadric $\mathcal{Q}$ and they give an accurate approximation of the true price only if an optimization over x is performed. Our contribution is to provide a new algorithm for solving both the optimization problems, that can be highly non trivial. The lower bound has a unique maximum when the log-correlations are all non negative and for this situation we provide a deterministic fast numerical scheme which converges to the maximum. When asset's correlations are negative, the lower bound can show multiple maxima and we propose an hybrid algorithm on two stages. First we use the Simulated Annealing for selecting the "right" zone near the global maximum and then we use the previous deterministic algorithm for reaching it with the desired level of accuracy.
The upper bound minimization problem is intrinsically highly non trivial because of the presence on n points, namely the n columns of the correlation matrix, where n is the dimension of the basket, in which the ICUB is not differentiable. These points in most of the cases are the solution of the optimization problem and therefore gradient methods for optimization may fail. The numerical scheme we propose for this problem is the hybrid scheme in which we first run the Simulated Annealing and then the deterministic fast map which does not suffer the non regularity of the columns of the correlation matrix.
Finally we perform numerical examples to test the performance of our algorithm compared standard optimization schemes.

References

[1] Lord, R. 2006 *Valuing Asian and portfolio options by conditioning on the geometric mean price.* J. Comput. Finan. 10, 1–42

[2] Kaas, R. et al. 2000 *Upper and lower bounds for sums of random variables.* Insurance: Mathematics and Economics 27, 151-168.

Forecasting with Dynamic Factor Models in both finite and infinite dimensional factor spaces

Fabio Della Marra
Università degli Studi di Parma
via J. F. Kennedy, 6 43125 - Parma Italy
fabio.dellamarra@iispascal.it

In this talk, we show a comparative analysis of the pseudo real-time forecasting performance of three Large-Dimensional Dynamic Factor Models. Large-Dimensional Dynamic Factor Models represent each variable in a dataset as decomposed into a *common component*, driven by a small (as compared to the number of series in the dataset) number of common factors, and an *idiosyncratic component*. The latter is assumed to be orthogonal or, at most, weakly correlated with respect to the different common factors, so that the covariance of the variables in the dataset is mostly accounted for by the common components. Typically, the asymptotic results are obtained for n, the number of series, and T, the number of observations for each series, both tending to infinity. Among the different versions of the Dynamic Factor Model we selected:

(i) The *SW model*. This model has been introduced in [1]. The factors are estimated by means of the standard Principal Components of the variables in the dataset. The forecast of the variable of interest, call it y_t, is obtained by regressing y_{t+h} on the factors and the variable y_t, plus possibly lags of the factors and y_t.

(ii) The *FHLR model*. It is a variant of the previous model which has been proposed in [2]. In a first step, the covariances of the common and of the idiosyncratic components are estimated using a frequency-domain method introduced in [3]. In the second step, such covariances are employed to estimate the factors by means of Generalized Principal Components.

(iii) The *FHLZ model*. Both models (i) and (ii) assume that the space spanned by the common components at any time t stays finite-dimensional as n tends to infinity. In [4], [5], it is assumed that a finite number of common shocks drive the common components, though the common components themselves are allowed to span an infinite-dimensional space. The dynamic relationship between the variables and the factors in this model is more general as compared to (i) and (ii). However, its estimation is rather complex and no systematic comparison with (i) and (ii) has as yet been produced.

We employ a large macroeconomic dataset consisting of 176 EU macroeconomic and financial time series observed at monthly frequency over the period from February 1986 to October 2015. To achieve stationarity, the series are desasonalized and transformed into first difference of the logarithm (mainly real variables), first difference of yearly difference of the logarithm (prices and wages), first difference (interest rates). A few stationary series are taken in levels. No treatment for outliers is applied.
A distinctive feature of our exercise is that we split our sample into a fairly large subsample, from February 1986 to December 2000, upon which different models of each class of models

(i), (ii), (iii) are calibrated to produce forecasts within the sample of the variables of the dataset. Then, for each class of models (i), (ii), (iii), we select the one which shows minimum mean square forecast error (MSFE). The selected models are then run and compared in the remaining sample, from January 2001 to October 2015. To generalize our results, we also test different sizes of the rolling window to conduct a robustness analysis.

References

[1] Stock, J. H. and Watson, M. W. (2002a). Forecasting using principal components from a large number of predictors. *Journal of the American Statistical Association*, 97(460):1167–1179.

[2] Forni, M., Hallin, M., Lippi, M., and Reichlin, L. (2005). The generalized dynamic factor model: One-sided estimation and forecasting. *Journal of the American Statistical Association*, 100:830–840.

[3] Forni, M., Hallin, M., Lippi, M., and Reichlin, L. (2000). The generalized dynamic-factor model: Identification and estimation. *Review of Economics and Statistics*, 82(4):540–554.

[4] Forni, M., Hallin, M., Lippi, M., and Zaffaroni, P. (2015). Dynamic factor model with infinite dimensional factor space: representation. *Journal of Econometrics*, 185:359–371.ù

[5] Forni, M., Hallin, M., Lippi, M., and Zaffaroni, P. (2016). Dynamic factor model with infinite dimensional factor space: Asymptotic analysis. EIEF Working Paper 2016/07, Einaudi Institute for Economics and Finance.

Option pricing and implied volatility estimation in jump-diffusion models: a Mellin transform approach

Marianito Rodrigo
University of Wollongong
Wollongong, NSW, Australia, 2522
marianito_rodrigo@uow.edu.au

T. Ray Li
University of Wollongong
Wollongong, NSW, Australia, 2522
tl115@uowmail.edu.au

We use Mellin transforms to derive alternative results for option pricing and implied volatility estimation when the underlying asset price is governed by jump-diffusion dynamics. The current well-known results are restrictive since the jump is assumed to follow a predetermined distribution (e.g., lognormal or double exponential). However, the results we present are general since we do not specify a particular jump-diffusion model within the derivations. In particular, we construct and derive an exact solution to the option pricing problem in a general jump-diffusion framework via Mellin transforms. This approach of Mellin transforms is further extended to derive a Dupire-like partial integro-differential equation, which ultimately yields an implied volatility estimator for assets subjected to instantaneous jumps in the price. Numerical simulations are provided to show the accuracy of the estimator. This talk is based on the article [1].

References

[1] T. Ray Li and Marianito R. Rodrigo (2016), Alternative results for option pricing and implied volatility in jump-diffusion models using Mellin transforms, submitted.

Advances in Quantitative Finance - Part II: numerical techniques

PROPOSERS

Chiara Guardasoni
Dip. di Matematica e Informatica, Università degli Studi di Parma
Parco Area delle Scienze, 53/A 43124 - Parma Italy
chiara.guardasoni@unipr.it

Daniele Marazzina
Dip. di Matematica, Politecnico di Milano
Via Bonardi, 9 20133 - Milano Italy
daniele.marazzina@polimi.it

Simona Sanfelici
Dip. di Economia, Università degli Studi di Parma
Via Kennedy, 6 43125 - Parma Italy
simona.sanfelici@unipr.it

SPEAKERS

Marzia Bisi
Dip di Matematica e Informatica, Università degli Studi di Parma
marzia.bisi@unipr.it

Chiara Guardasoni
Dip. di Matematica, Università degli Studi di Parma
chiara.guardasoni@unipr.it

Gaetano La Bua
Dip. di Matematica, Politecnico di Milano
gaetano.labua@polimi.it

Daniele Marazzina
Dip. di Matematica, Politecnico di Milano
daniele.marazzina@polimi.it

Giulia Livieri
Scuola Normale Superiore di Pisa
giulia.livieri@sns.it

Antonino Zanette
Dip. di Scienze Economiche e Statistiche, Università degli Studi di Udine
antonino.zanette@uniud.it

In recent years the research for mathematical tools to be applied in financial contexts has gained additional importance. In fact the latest financial crisis has highlighted the need for a more scientific approach to the problem of pricing and risk control. Moreover,

we can now take advantage of more advanced statistical and mathematical skills and of the availability of numerical techniques and faster computer systems.

In this minisymposium, a variety of advanced mathematical modelling tools, numerical methods and scientific computation techniques for different current problems in quantitative finance will be presented. More precisely, this second part of the minisymposium is devoted to present recent contributions of numerical techniques in solving financial problems.

A kinetic approach to simple market economies

Marzia Bisi
Università degli Studi di Parma
Parco Area delle Scienze, 53/A 43124 - Parma, Italy
marzia.bisi@unipr.it

Giampiero Spiga
Università degli Studi di Parma
Parco Area delle Scienze, 53/A 43124 - Parma, Italy
giampiero.spiga@unipr.it

Giuseppe Toscani
Università degli Studi di Pavia
Via Ferrata, 1 27100 - Pavia, Italy
giuseppe.toscani@unipv.it

In recent years, kinetic equations of Boltzmann type have been proposed to model simple open market economies, based on the idea that an economic system composed by a sufficiently large number of agents can be described using the laws of statistical mechanics as it happens in a physical system composed of many interacting particles. The details of the economical interactions between agents characterize their wealth distribution. The features typically incorporated in kinetic trade models are saving effects and randomness: saving means that each agent is guaranteed to retain at least a certain minimal fraction of his initial wealth at the end of the trade; randomness means that the amount of money changing hands is non–deterministic. A substantial difference on the final behavior of the model can be observed depending on the fact that binary trades are pointwise conservative [3], or conservative in the mean [4]; indeed, the presence of suitable random variables allows to identify steady profiles with proper "Pareto tails", namely asymptotic to an inverse power of wealth. The major results about kinetic equations for multi–agent systems have been summarized in the book [5].
In this talk, we propose a new class of kinetic equations in which agent's trading propensity varies according to the personal amount of wealth [1], and we discuss the distribution behavior in suitable asymptotic limits, comparing the results with the ones available for simpler models. Moreover, we present a kinetic approach taking into account, besides the effects of binary interactions and of market risk, other non–negligible phenomena in real economy such as taxation and redistribution of the collected wealth [2]. The taxation mechanism is introduced at the level of the single trade to generate a portion of the mean wealth of the society, that will be totally redistributed to agents, to maintain the total wealth constant. The mechanism of redistribution is assumed sufficiently flexible to be able to redistribute to agents a constant amount of wealth independently of the wealth itself, or to redistribute proportionally (or inversely proportionally) to their wealth. In suitable asymptotic regimes, in terms of various parameters involved in the model, the kinetic Boltzmann equation turns out to be well approximated by a Fokker–Planck–type equation, which may be solved in order to determine the crucial properties of its steady state.

References

[1] Bisi, M. 2016 *Some kinetic models for a market economy* (submitted).

[2] Bisi, M., Spiga, G. and Toscani, G. 2009 *Kinetic models of conservative economies with wealth redistribution*. Commun. Math. Sci. 4, 901–916.

[3] Chakraborti, A. and Chakrabarti, B.K. 2000 *Statistical mechanics of money: How saving propensity affects its distribution*. Eur. Phys. J. B 17, 167–170.

[4] Cordier, S., Pareschi, L. and Toscani, G. 2005 *On a kinetic model for a simple market economy*. J. Stat. Phys. 120, 253–277.

[5] Pareschi, L. and Toscani, G. 2014 *Interacting Multiagent Systems: Kinetic Equations and Monte Carlo Methods*. Oxford University Press.

A Boundary Element Method applied to Barrier Options Pricing

Chiara Guardasoni
Università degli Studi di Parma
viale Parco Area delle Scienze, 53/A 43124 - Parma Italy
chiara.guardasoni@unipr.it

Simona Sanfelici
Università degli Studi di Parma
via Kennedy, 6 43125 - Parma Italy
simona.sanfelici@unipr.it

The recent financial crisis has highlighted the need for a more scientific approach to the problem of pricing and risk control, taking advantage of more advanced statistical and mathematical skills and of the availability of numerical techniques and faster computer systems.
European options are derivative contracts that give the buyer the right to buy/sell a particular asset at a fixed maturity, at a predetermined price. In the case of "barrier option", this right gets into existence or extinguishes when the underlying asset reaches a certain barrier value.
The Black-Scholes model (BS) [2] can be considered the first of the differential models for option pricing. Over the past three decades, the academic literature has highlighted the strong limitations of this model due to the fact that it is based on restrictive and unrealistic assumptions. Therefore other methods have been later introduced:

- models with time-dependent parameters or models where the volatility of the asset is a deterministic function of price and time;
- stochastic volatility models, such as the Heston model [5], in which the value of the option depends on time, on the price and on the volatility of the underlying asset;
- jump-diffusion models, such as the Bates model [1], that involves the adoption of stochastic processes with jumps in the analysis of fluctuations of financial markets.

For these more advanced models, the pricing of "barrier option" is traditionally based on Monte Carlo methods that are affected by high computational costs and inaccuracy due to their slow convergence or on domain methods (such as Finite Element Methods and Finite Difference methods) that have some troubles particularly in unbounded domains.
Recently, at the University of Parma, a stable, accurate and efficient numerical method has been developed for the BS with time-constant parameters [3] and for Heston and Bates models [4].
The new approach is based on the Boundary Element Method (BEM) that was introduced in the Engineering field in 1970. The method is particularly advantageous for its high accuracy, for the implicit satisfaction of the asymptotic conditions at infinity and for the low discretization costs, especially when the differential problem is defined in an unbounded domain and the data are assigned on a limited boundary (which is the case of

the "barrier option").
Here the method is illustrated with some adaptations in order to solve the pricing problem of an up-and-out put option in the BS model with time-dependent parameters. Note that the explained procedure is absolutely general and it can be followed also when considering European call options with different single or double barriers (down/up, in/out) just resulting in different initial/boundary conditions for the starting differential problem but that can be treated in the same way.

References

[1] Bates, D. 1996, *Jumps and stochastic volatility: exchange rate processes implicit in Deutsche mark options*. Review of Financial Studies, 9, 69–107.

[2] Black, F. and Scholes, M. 1973, *The Pricing of Options and Corporate Liabilities*. Journal of Political Economy, 81(3), 637–654, .

[3] Guardasoni, C. and Sanfelici, S. 2016, *A boundary element approach to barrier option pricing in Black-Scholes framework*. International Journal of Computer Mathematics, 93(4), 696–722.

[4] Guardasoni, C. and Sanfelici, S. 2016, *Fast Numerical Pricing of Barrier Options under Stochastic Volatility and Jumps*. SIAM J. Appl. Math, 76(1), 27–57.

[5] Heston, S.L. 1993, *A closed-form solution for options with stochastic volatility with applications to bond and currency options*, Review of Financial Studies, 6, 327–343.

Matrix Processes in Derivatives Pricing: Modelling and Numerical Techniques

Gaetano La Bua
Politecnico di Milano Piazza Leonardo da Vinci, 32 20133 - Milano Italy
gaetano.labua@polimi.it

There is an empirical evidence that the dynamics of the implied volatility surface is driven by several factors. This causes the standard one-factor stochastic volatility models not to be flexible enough to consistently price plain vanilla options and forward volatility sensitive derivatives (e.g. forward starting and cliquet options). It is well accepted that a multi-factor approach would be necessary to take into account the variability of the skew. A large part of existing literature has considered vector-valued stochastic processes to model the multidimensional stochastic evolution of asset volatility. The choice of $\mathbb{R}^n$ as state space for the volatility process, however, could lead to unsatisfactory dependence structures among variance factors. This is particularly true if we restrict ourselves to the case of affine processes. In the light of the above, it appears reasonable to consider more general multidimensional processes: recently an increasing attention has been devoted to applications of matrix-defined stochastic processes in derivatives pricing. In particular, stochastic processes defined on the cone of positive semidefinite matrices $\mathcal{S}_n^+$ can be seen as natural candidates to model the latent volatility factors.
In this talk we focus on the so-called Wishart processes introduced by Bru [2] as a matrix generalization of square-root processes. A remarkable feature is that the analytical tractability is fully preserved since they belongs to the class of affine processes. Given the strict connection with the well-known CIR processes, Wishart processes have been used to define multi-factor [4] and multi-asset [3] extensions of the classic Heston model. Despite the analytical tractability, the implementation of Wishart-based stochastic volatility models poses non-trivial challenges from a numerical point of view. Firstly, we present simple and efficient simulation schemes for the asset price trajectories, making use of the exact sampling scheme in [1], that allow to price path-dependent derivatives. Secondly, we discuss the calibration problem and we highlight the constraints that need to be satisfied in order to get a well-defined Wishart process. Lastly, we introduce a wider class of hybrid models that improves the accuracy in reproducing the market volatility surface.

References

[1] Ahdida, A. and Alfonsi, A. 2013 *Exact and high-order discretization schemes for Wishart processes and their affine extensions*. The Annals of Applied Probability, vol. 212, no. 3, 1025–1073.

[2] Bru, M. 1991 *Wishart processes*. Journal of Theoretical Probability, vol. 4, no. 4, 725–751.

[3] Da Fonseca, J., Grasselli, M. and Tebaldi, C. 2007 *Option pricing when correlations are stochastic: an analytical framework*. Review of Derivatives Research, vol. 10, no. 2, 151–180.

[4] Da Fonseca, J., Grasselli, M. and Tebaldi, C. 2008 *A multifactor volatility Heston model*. Quantitative Finance, vol. 8, no. 6, 591–304.

Spitzer Identity, Wiener-Hopf Factorization and Pricing of Discretely Monitored Exotic Options

Daniele Marazzina
Politecnico di Milano
Piazza Leonardo da Vinci, 32 - 20133 Milano, Italy
daniele.marazzina@polimi.it

Gianluca Fusai
Università del Piemonte Orientale "Amedeo Avogadro"
Via Perrone, 18 - 28100 Novara, Italy
gianluca.fusai@unipmn.it

Guido Germano
University College London
Gower Street - London, UK
g.germano@ucl.ac.uk

The Wiener-Hopf factorization of a complex function arises in a variety of fields in applied mathematics such as probability, finance, insurance, queuing theory, radio engineering and fluid mechanics. The factorization fully characterizes the distribution of functionals of a random walk or a Lévy process, such as the maximum, the minimum and hitting times. Here we propose a constructive procedure for the computation of the Wiener-Hopf factors, valid for both single and double barriers, based on the combined use of the Hilbert and the z-transform. The numerical implementation can be simply performed via the fast Fourier transform and the Euler summation. Given that the information in the Wiener-Hopf factors is strictly related to the distributions of the first passage times, as a concrete application in mathematical finance we consider the pricing of discretely monitored exotic options, such as lookback and barrier options, when the underlying price evolves according to an exponential Lévy process. We show that the computational cost of our procedure is independent of the number of monitoring dates and the error decays exponentially with the number of grid points.

More precisely, this work provides a new procedure to determine the finite-time distribution of the discrete extrema and of the hitting times of one or two barriers for a process with independent and identically distributed increments, such as a Lévy process. Spitzer [2] provided a closed formula for the z-transform (or moment generating function or discrete Laplace transform) of the characteristic function of the extrema of a random walk observed on a set of discrete dates. Up to now the concrete application of the Spitzer identity has been difficult because it requires the Wiener-Hopf (WH) factorization of a function defined in the complex plane, a mathematical problem that concerns a variety of fields in applied mathematics. Indeed, this factorization cannot be achieved analytically except in few cases, or its computation turns out to be very demanding requiring the numerical evaluation of a multidimensional integral in the complex plane. In addition, with regard to a general Lévy process, little is known for the two-barriers case.
The key contributions of our work are the following. First of all, we provide a constructive

procedure for performing the WH factorization. More precisely, we express the WH factors arising in the Spitzer identity in terms of the Plemelj-Sokhotsky relations, which allow us to compute the WH factors through the Hilbert transform. The latter is then approximated via a sinc function expansion [3], which guarantees an exponential decay of the approximation error on the number of grid points.
Moreover, our methodology can deal with both a single and a double barrier. The solution in the second case is of interest in itself because it solves a long-standing problem related to an efficient computation of the WH factors in the presence of two barriers. The double-barrier case did not admit a simple feasible solution up to now, except under few special assumptions on the structure of the Lévy process. One has to solve two coupled integral equations, which can be achieved by factorizing a 2×2 matrix of functions, but a general analytical method for this more difficult problem has not been found yet [1]. Here, as the second main contribution of the work, we constructively propose a fixed-point algorithm based on an extension of the single-barrier case that achieves a fast convergence.

References

[1] Jones, D. S. 1991 Wiener-Hopf splitting of a 2×2 matrix. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences 434, 419–433.

[2] Spitzer, F. 1956 A combinatorial lemma and its application to probability theory. Transactions of the American Mathematical Society. 82(2), 323–339.

[3] Stenger, F. 1993 *Numerical Methods Based on Sinc and Analytic Functions*. Springer.

A backward Monte Carlo approach to exotic option pricing

Giulia Livieri
Scuola Normale Superiore,
Piazza dei Cavalieri, 7 56126 - Pisa Italy
giulia.livieri@sns.it

Giacomo Bormetti
Università di Bologna
Piazza di Porta San Donato, 5 40126 - Bologna Italy
giacomo.bormetti@unibo.it

Giorgia Callegaro
Università degli Studi di Padova
Via Trieste, 63 35121 - Padova Italy
gcallega@unipd.it

Andrea Pallavicini
Department of Mathematics, Imperial College
London SW7 2AZ, United Kingdom
a.pallavicini@imperial.ac.uk

We propose a novel algorithm – termed backward Monte Carlo – to the Monte Carlo simulation of continuous time diffusion processes. The new algorithm exploits recent advances in the quantization of diffusion processes ([Pagès(2014)], [Pagès et al.(2004)], [Pagès & Printems(2003)]) to approximate the continuous process with a discrete-time Markov Chain defined on a finite grid of points. Specifically, we consider the Recursive Marginal Quantization Algorithm ([Pagès & Sagna(2013)], [Callegaro et al.(2015)]), and as a first contribution we investigate a fixed-point scheme – termed Lloyd I method ([Kieffer(1982)]) with Anderson acceleration ([Anderson(1965)]) – to compute the optimal grid in a robust way. As a complementary approach, we consider the grid associated with the explicit scheme approximation of the Markov generator of a piecewise constant volatility process ([Albanese(2007)], [Albanese & Mijatović(2007)]). The latter approach – termed Large Time Step Algorithm – turns out to be competitive in pricing payoff specifications which require the observation of the price process over a finite number of pre-specified dates. Both methods – quantization and the explicit scheme – provide us with the marginal and transition probabilities associated with the points of the approximating grid. Sampling from the discrete grid backward – from the terminal point to the spot value of the process – in a similar spirit to the Brownian Bridge ([Glasserman(2003)]) we design a simple but effective mechanism to draw Monte Carlo path and achieve a sizeable reduction of the variance associated with Monte Carlo estimators. Our conclusion is extensively supported by numerical experiments.

References

[Albanese(2007)] Albanese, C. (2007) Operator methods, abelian processes and dynamic conditioning. *Abelian Processes and Dynamic Conditioning (October 16, 2007)*.

[Albanese & Mijatović(2007)] Albanese, C. & Mijatović, A. (2007) Convergence Rates for Diffusions on Continuous-Time Lattices. Working paper.

[Anderson(1965)] Anderson, D.G. (1965) Iterative procedures for nonlinear integral equations. *Journal of the ACM (JACM)* **12(4)**, 547–560.

[Callegaro et al.(2015)] Callegaro, G. & Fiorin, L. & Grasselli, M. (2015) Quantized calibration in local volatility. *Risk Magazine*.

[Glasserman(2003)] Glasserman, P. (2003) *Monte Carlo methods in financial engineering*. Springer Science & Business Media.

[Kieffer(1982)] Kieffer, J.B. (1982) Exponential rate of convergence for Lloyd's method I. *Information Theory, IEEE Transactions on* **28(2)**, 205–210.

[Pagès(2014)] Pagès, G. (2014) Introduction to optimal vector quantization and its applications for numerics. Preprint.

[Pagès et al.(2004)] Pagès, G. & Pham, H. & Printems, J. (2004) Optimal quantization methods and applications to numerical problems in finance. *Handbook of computational and numerical methods in finance*, 253–297.

[Pagès & Printems(2003)] Pagès, G. & Printems, J. (2003) Optimal quadratic quantization for numerics: the Gaussian case. *Monte Carlo Methods and Applications* **9(2)**, 135–165.

[Pagès & Sagna(2013)] Pagès, G. & Sagna, A. (2013) Recursive marginal quantization of an Euler scheme with applications to local volatility models. Preprint.

Hybrid tree-finite difference methods for the Heston and Bates model with stochastic interest rates

Antonino Zanette
Università di Udine
via Tomadini, 30 33100 - Udine Italy
antonino.zanette@uniud.it

Maya Briani
Istituto per le Applicazioni del Calcolo, CNR Roma
m.briani@iac.cnr.it

Lucia Caramellino
Università di Roma Tor Vergata
caramell@mat.uniroma2.it

We propose a mixed tree-finite difference method in order to approximate the Heston model. We prove the convergence by embedding the procedure in a bivariate Markov chain. Moreover, as a by-product, we provide a new simulation scheme to be used for Monte Carlo evaluations. Numerical results show reliability and the efficiency of the algorithms. We show how to generalize the procedure to the Bates model, the Heston-Hull-White model and the Heston-Hull-White2D model.

Analysis and numerics for the modeling through conservation laws

PROPOSERS

Graziano Guerra
Università degli Studi di Milano–Bicocca
Dip. di Matematica e Applicazioni - Via Cozzi, 55 - 20125 Milano
graziano.guerra@unimib.it

Francesca Marcellini
Università degli Studi di Milano–Bicocca
Dip. di Matematica e Applicazioni - Via Cozzi, 55 - 20125 Milano
francesca.marcellini@unimib.it

SPEAKERS

Andrea Corli
Dip. di Matematica e Informatica, Università degli Studi di Ferrara,
andrea.corli@unife.it

Carlotta Donadello
Laboratoire de Mathématiques, Université de Franche-Comté, Besançon Cedex, France,
Carlotta.Donadello@univ-fcomte.fr

Mauro Garavello
Dip. di Matematica e Applicazioni, Università di Milano–Bicocca
mauro.garavello@unimib.it

Paola Goatin
INRIA Sophia Antipolis
paola.goatin@inria.fr

Elena Rossi
Dip. di Matematica e Applicazioni, Università di Milano–Bicocca
e.rossi50@campus.unimib.it

Laura V. Spinolo
CNR-IMATI: Pavia
laura.spinolo@imati.cnr.it

The fundamental progresses achieved in recent years by the mathematical theory of hyperbolic conservation laws has made possible the study of several applied and physical phenomena. The aim of this Minisymposium is to consider some of these new problems from both the analytic and applicative point of view. The problems we consider range over traffic flow, boundary layers for Navier–Stokes equations, hyperbolic models for hysteresis, inverse/control problems. In particular in the context of traffic flow the following problems will be analyzed: models on both unidirectional roads and networks, L^1 dissipative solver for traffic junctions, moving bottleneck, two phase models on networks. The speakers

in this Minisymposium have a deep competence in the study of hyperbolic systems of conservation laws, hyperbolic equations with nonlocal flux, mixed systems PDE-ODE and conservation laws on networks. This competence extends to the analytical and numerical study of this kind of systems as well as to their application to several applied problems.

Two-modes flow in porous media with hysteresis

Andrea Corli
University of Ferrara
via Machiavelli, 30 450121 - Ferrara Italy
andrea.corli@unife.it

Haitao Fan
Georgetown University
Washington D.C. 20057 U.S.A.
fan@math.georgetown.edu

This paper focuses on a very simple model of hysteresis arising in oil recovery that was proposed in [2]. We consider a fluid flow in a porous medium, which is constituted by a water phase and an oil phase. The flow is modeled by the diffusive equation

$$s_t + f_x = \epsilon s_{xx}, \tag{1}$$

where s is the water saturation, f the water fractional flow and ϵ the capillarity-induced diffusion coefficient. Both s and f are valued in $[0, 1]$. Hysteresis comes into the play through the flow f, which does not only depend on s but also on its history and current trend. Therefore, the flow f can be thought as a multi-valued function; for s fixed, these multiple values are parametrized by a new variable π, which encodes the behavior of s in the past and the actual increasing or decreasing of s. As a consequence, an equation for π is introduced.
In the case $\epsilon = 0$, the Riemann problem for equation (1) was sketched in [2]. The solution to such problem is far from being unique, not only because many combination of waves are possible for the same initial data, but in particular because hysteresis loops appear. However, for constant $\epsilon > 0$, a relaxation approximation for the equation of π is introduced in [2] and the authors determine which shock waves have a diffusive-relaxation profile. The drawback of this construction is that the flux function needs to be extended outside its natural domain, as well as the solutions.
In this talk we avoid introducing relaxation. First, we describe which waves admit viscous profiles. Then, we introduce the notion of weak solution for the initial-value problem for (1). At last, we introduce a Riemann solver for the inviscid ($\epsilon = 0$) system and discuss its uniqueness. Complete details are provided in [1].

References

[1] Corli, A., and Fan, H. 2016 *Two-modes flow in porous media with hysteresis.* Preprint.

[2] Plohr, B., Marchesin, D., Bedrikovetsky, P. and Krause, P. 2001 *Modeling hysteresis in porous media flow via relaxation.* Comput. Geosci. 5, 225-256.

Well-posedness for a monotone solver for traffic junctions

Carlotta Donadello
Laboratoire de Mathématiques
Université de Franche-Comté
16 route de Gray
25030 Besançon Cedex - France
carlotta.donadello@univ-fcomte.fr

Boris P. Andreianov
Laboratoire de Mathématiques et Physique Théorique
Université de Tours
Parc de Grandmont
37200 Tours - France
Boris.Andreianov@lmpt.univ-tours.fr

Giuseppe M. Coclite
Dipartimento di Matematica
Università degli Studi di Bari
Via Orabona 4
70125 Bari - Italy
giuseppemaria.coclite@uniba.it

In this talk we present well-posedness results for solutions obtained as vanishing viscosity limits for the Cauchy problem on a traffic junction where m incoming and n outgoing roads meet. We assume that the traffic on each road is governed by a scalar conservation law like in the classical LWR model.
Our proof relies on the introduction of a family of Kruzhkov-type adapted entropies at the junction and a suitable definition of admissible solution.
The key step in our construction consists in the description and analysis of the set of stationary solutions for the inviscid problem from the point of view developed by Andreianov, Karlsen, Risebro and Cancès to deal with scalar conservation laws with discontinuous flux.

A phase-transition model for traffic at junctions

Mauro Garavello
Dipartimento di Matematica e Applicazioni
Università degli Studi di Milano Bicocca
via R. Cozzi, 55 20125 - Milano Italy
mauro.garavello@unimib.it

Francesca Marcellini
Dipartimento di Matematica e Applicazioni
Università degli Studi di Milano Bicocca
via R. Cozzi, 55 20125 - Milano Italy
francesca.marcellini@unimib.it

We consider the phase-transition model for traffic, introduced by Colombo, Marcellini and Rascle in [1], and we extend it to the case of junctions. We propose a solution at junctions, which preserves the number of cars and distributes the maximal speed of each vehicle according to the flux distribution. Properties of the Riemann solvers at junctions will be presented.

References

[1] R. M. Colombo, F. Marcellini, M. Rascle, *A 2-phase traffic model based on a speed bound*, SIAM J. Appl. Math. **70** (2010), no. 7, 2652–2666.

A Riemann Solver at junctions preserving priorities

Paola Goatin
Inria Sophia Antipolis Méditerranée
2004, route des Lucioles - BP 93, 06902 Sophia Antipolis Cedex, FRANCE
paola.goatin@inria.fr

Maria Laura Delle Monache
Department of Mathematical Sciences, Rutgers University - Camden
227 Penn St, Camden, NJ 08102, USA
ml.dellemonache@rutgers.edu

Benedetto Piccoli
Department of Mathematical Sciences and CCIB, Rutgers University - Camden
311 N 5th Street, Camden, NJ 08102, USA
piccoli@camden.rutgers.edu

Traffic flow on road networks, represented as directed graphs, can be described by conservation laws accounting for traffic evolution on each arc and coupled by suitable conditions at junctions. This amounts at prescribing specific solvers for the Riemann problems at nodes, i.e. Cauchy problems corresponding to constant initial conditions on each incoming and outgoing edge.
The first results concerning Lighthill-Whitham-Richards model on networks is due to Holden and Risebro [5], who proposed a solution choice based on the maximisation of the flux through the junction. In [1], some fixed rules for the distribution of traffic plus optimization criteria for the flux are prescribed. In particular, conditions guaranteeing uniqueness of solutions exclude junctions with more incoming than outgoing roads. We refer to [3] for further details and references.
Here we present a new general Riemann solver at junctions based on flux maximisation subject to traffic distribution rules among outgoing roads and priority rules among incoming roads. In particular, the Riemann problem exhibit unique solutions for any number of incoming and outgoing roads.
We also give a general existence result for the Cauchy problem with initial data with bounded total variation, based on the fulfilment of some properties controlling the increase of the total variation of the flux, inspired by [4]. In particular, we prove existence of solutions corresponding to our Riemann solver in the case of 2×2 junctions [2].

References

[1] G.M. Coclite, M. Garavello, and B. Piccoli. Traffic flow on a road network. *SIAM J. Math. Anal.*, 36(6):1862–1886, 2005.

[2] M. L. Delle Monache, P. Goatin, and B. Piccoli. Priority-based Riemann solver for traffic flow on networks. In preparation.

[3] M. Garavello and B. Piccoli. *Traffic flow on networks*, volume 1 of *AIMS Series on Applied Mathematics*. American Institute of Mathematical Sciences (AIMS), Springfield, MO, 2006. Conservation laws models.

[4] M. Garavello and B. Piccoli. Conservation laws on complex networks. *Ann. I. H. Poincaré*, 26:1925–1951, 2009.

[5] Helge Holden and Nils Henrik Risebro. A mathematical model of traffic flow on a network of unidirectional roads. *SIAM J. Math. Anal.*, 26(4):999–1017, 1995.

IBVPs for Hyperbolic Balance Laws with Applications to Traffic Modelling

Elena Rossi
Università degli Studi di Milano – Bicocca
via R. Cozzi 55 - 20125 Milano Italy
e.rossi50@campus.unimib.it

Rinaldo M. Colombo
Università degli studi Brescia
Via Branze 38 - 25123 Brescia Italy
rinaldo.colombo@unibs.it

Conservation and balance laws are at the basis of a variety of models of interest, for instance, in industry or in biology, see [2]. Often, these models naturally require to be set in suitable bounded domains. In this talk, we first overview recent analytic results [3] developed on the basis of the classical work [1], concerning balance laws with boundaries in several space dimensions. Then, we specialize these statements in a 1D non autonomous setting suitable for applications to traffic dynamics, aiming in particular at the optimal management of traffic flows. Indeed, the recent results in [4] ensure the stability with respect to the flow of solutions to an IBVP for a scalar conservation law.

References

[1] C. Bardos, A. Y. le Roux, and J.-C. Nédélec. First order quasilinear equations with boundary conditions. *Comm. Partial Differential Equations*, 4(9):1017–1034, 1979.

[2] R. M. Colombo, F. Marcellini, and E. Rossi. Biological and industrial models motivating nonlocal conservation laws: a review of analytic and numerical results. *Netw. Heterog. Media*, 11(1):49–67, 2016.

[3] R. M. Colombo and E. Rossi. Rigorous estimates on balance laws in bounded domains. *Acta Math. Sci. Ser. B Engl. Ed.*, 35(4):906–944, 2015.

[4] R. M. Colombo and E. Rossi. Stability of the 1D IBVP for a non autonomous scalar conservation law. Preprint, 2016.

On the local limit of continuity equations with nonlocal fluxes.

Laura V. Spinolo
IMATI-CNR
via Ferrata 1, I-27100 Pavia Italy
spinolo@imati.cnr.it

Stefano Bianchini
SISSA
via Bonomea 265, I-34136, Trieste, Italy
bianchin@sissa.it

Maria Colombo
Universität Zürich
Winterthurerstrasse 190, CH-8057 Zürich, Switzerland
maria.colombo@math.uzh.ch

Gianluca Crippa
Universität Basel
Spiegelgasse 1, CH-4051 Basel, Switzerland
gianluca.crippa@unibas.ch

Consider a family of continuity equations where the velocity field is given by the convolution of the solution with a regular kernel. In the singular limit where the convolution kernel is replaced by a Dirac delta, one formally recovers a conservation law. My talk will aim at discussing the behavior of the solutions of the nonlocal continuity equation in the singular limit. I will recall some positive results and discuss some recent counter-examples. I will also discuss the nonlocal to local limit for a related family of continuity equations with a viscous second order term.

Computational methods in algebraic and analytical models

PROPOSERS

Maurizio Imbesi
Università degli Studi di Messina
maurizio.imbesi@unime.it

Monica La Barbiera
Università degli Studi di Catania

Paola Lea Staglianò
Università degli Studi di Palermo

SPEAKERS

Gioia Failla
Dip. IIES, Università di Reggio Calabria
gioia.failla@unime.it

Monica La Barbiera
Dip. Ingegneria Industriale, Università di Catania
monicalb@libero.it

Paola Lea Staglianò
Dip. ICAM, Università di Palermo
paolalea.stagliano@unipa.it

Anna Maria Stanganelli
Dip. MI, Università di Palermo
annamaria.stanganelli@unipa.it

Maurizio Imbesi
Università degli Studi di Messina
Viale F. Stagno d'Alcontres, 31 98166 - Messina Italy
imbesim@unime.it

Mario Versaci
Dip. ICEAM, Università di Reggio Calabria
mario.versaci@unirc.it

The present minisymposium explains how commutative and computational algebra, linear and non-linear algebra, algebraic graph theory and combinatorics could help applied science for giving solutions on real problems concerning different sectors. The proposal covers recent developments dealing with these topics in order to translate or evaluate theoretic results into concrete realities.
Algebraic and analytical models are becoming increasingly significant because they are directed to other areas of sciences and technology. They are being actively considered in

various fields such as physical, statistical, medical ones and in biochemistry, engineering, computer science, and so on.
For example, models of this type are substantially given by graphs and matrices in algebraic systems. They are basically used to represent relations and processes in more contexts: telecommunication systems, interchange networks, transportation optimal plan of indivisible goods, microwave engineering in resonant structures, coding theory, data organization, flows of computation, research algorithms for the web, etc.
Algebraic and analytical models are a universal instrument for any kind of question that can be modeled by polynomial equations and also one of the most powerful methods in commutative algebra and algebraic geometry. The range of theoretical issues and applications related to them is enormous; it includes theoretical physics, computational graphic, electromagnetic parameters, and similar scientific layouts, since a lot of problems in such branches can be represented by algebra and numerical analysis (ideals, modules, matrices). For instance, the Groebner bases of toric ideals or those of hypersimplexes are an algebraic tool used by researchers in optimization problems, statistical processing, signal and image reshaping, computer vision science, and in the field of security to encrypt messages or to transmit confidential information.
The purpose of the minisymposium is that to collect recent experiences of researches for discussing several applications of mathematical models in different scientific areas.

Digraphs and Optimization Problems

Gioia Failla
University of Reggio Calabria
DIIES, Loc. Feo di Vito, 89122 - Reggio Calabria Italy
gioia.failla@unirc.it

In the study of problems about transportation problems of units of indivisible goods, we investigate on the digraphs associated to the $(1,1)$-Segre model consisting by the Segre product $A_{(1,1)} = K[x_1, \ldots, x_m] \otimes_S K[y_1, \ldots, y_n]$ of two polynomial rings in n and m variables on any field K. The model has good algebraic properties that reflect on the digraphs. Moreover the Groebner basis of the monomial algebra $A_{(1,1)}$ with respect a term order $<_\omega$, being $\omega \in N^{nm}$ a vector cost, it is very important to determine when the optimal transportation plan is unique and when a digraph has a unique sink.
We give examples of vectors cost not optimal, in correspondence of Groebner bases of the toric ideal of the model different from the usual Groebner bases used in [1],[2].
For low values of m and n, we resolve the problem of transportation problem in details, studying some fibers of the semigroup homomorphism that arises from the model and the associate digraphs having that fibers as support.

References

[1] Failla, G. 2014 *On the* $(1,1)$*-Segre Model for Business*, Applied Mathematical Sciences, Vol.8, n.166, 8329-8336

[2] Sturmfels, B 1995 *Groebner bases and convex polytopes*, Univ.Lect.Series, Vol.8, Amer.Math.Soc

Spanning trees of simple graphs

Monica La Barbiera
Università degli Studi di Messina
Viale F. Stagno d'Alcontres, 31 98166 - Messina Italy
monicalb@unime.it

Maurizio Imbesi
Università degli Studi di Messina
Viale F. Stagno d'Alcontres, 31 98166 - Messina Italy
imbesim@unime.it

Classes of simple graphs are studied using computational and algebraic methods in order to give geometrical models in real connection problems. In fact the models built through graph theory are useful for setting suitable solutions of several problems concerning network areas (infrastructure nets, circuits electrical workers, urban and territorial analysis, etc.).
Let $\mathcal{G}$ be a finite simple connected graph with the vertex set $V(\mathcal{G})$ and edge set $E(\mathcal{G})$, a spanning tree of $\mathcal{G}$ is a subgraph of $\mathcal{G}$ that contains every vertex of $\mathcal{G}$ and is also a tree. We represent the collection of all edge-sets of the spanning trees of $\mathcal{G}$ by $s(\mathcal{G})$:

$$s(\mathcal{G}) = \{E(G_i) \subset E(\mathcal{G}), \text{where } \ T_i \ \text{ is a spanning tree of } \ \mathcal{G}\}.$$

One can find a spanning tree systematically by cutting-down method, which says that spanning tree of a given simple finite connected graph is obtained by removing one edge from each cycle appearing in the graph.
We study some combinatorial properties of the spanning trees of Jahangir graphs. The *Jahangir graph* $J_{n,m}$, for $n \geq 2, m \geq 3$, is a graph on $nm + 1$ vertices consisting of a cycle C_{nm} with one additional vertex which is adjacent to m vertices of C_{nm} at distance n to each other on C_{nm}.
Our aim is to show how enumerate and describe all the spanning trees of a Jahangir graph $J_{n,m}$. More precisely we give an algorithm for the computation of the number of the spanning trees for this class of graphs.

References

[1] Anwar, I., Raza, Z. and Kashif A. 2015 *Spanning simplicial complexes of uni-cyclic graphs.* Alg. Colloq. 22(4), 707–710.

[2] Harary, F. 1994 *Graph Theory.* Reading, MA - Addison-Wesley.

[3] Lourdusamy, A., Jeyaseelan, S. S. and Mathivanan, T. 2015 *On pebbling Jahangir graph.* Gen. Math. Notes 5(2), 42–49.

Symmetric Algebras of Ideals Generated by Linear Forms

Paola Lea Staglianò
Università degli Studi di Palermo
Viale delle Scienze, Ed. 8 90128 - Palermo Italy
paolalea.stagliano@unipa.it

Gaetana Restuccia
Università degli Studi di Messina
Viale F. Stagno D'Alcontres, 31 98166 - Messina Italy
grest@unime.it

Let M be a finitely generated module on a commutative ring R with identity. Let $A = (a_{ij})$ be a $n \times m$ matrix, with entries in R, $I_k(A)$ the ideal generated by the $k \times k$ minors of A, $1 \leq k \leq \min(m, n)$, and let $\varphi : R^m \to R^n$ be a module homomorphism. We denote by $I_k(\varphi)$ the ideal $I_k(A)$, where $A = (a_{ij})$ is the $n \times m$ matrix associated to φ, for an appropriate choice of the bases.
Let

$$R^m \xrightarrow{\varphi} R^n \to M \to 0 \tag{1}$$

be a free presentation of the module M. If we consider the symmetric algebras of the modules in (1), the presentation ideal J of $Sym_R(M)$ is generated by the linear forms in the variables Y_j, $1 \leq j \leq n$:

$$a_i = \sum_{j=1}^{n} a_{ji} Y_j, \qquad 1 \leq i \leq m$$

The theory of $s-$sequences has been recently introduced by Herzog, Restuccia, Tang ([2]) and it permits to compute the invariants of $Sym_R(M)$ starting from the main algebraic invariants of quotients of R, via the initial ideal $\text{in}_<(J)$, with respect to a suitable term order, introduced in $R[Y_1, \ldots, Y_n]$, where n is the number of elements in a minimal system of generators of M.
We are interested to the case the ideal J is generated by an s-sequence. The problem is part of a wider context, precisely:
Given an ideal $I = (a_1, \ldots, a_m) \subset R[X_1, \ldots, X_n]$ generated by linear forms in the variables $X_1, \ldots, X_n$, we want to study when I is generated by an $s-$sequence and to compute the standard invariants of $Sym_R(I)$ in terms of the corresponding invariants of special quotients of the ringR.
Standard invariants of $Sym_R(I)$ are Krull dimension, multiplicity, depth and regularity, denoted respectively by $dim(Sym_R(I))$, $e(Sym_R(I))$, $depth(Sym_R(I))$ with respect to the maximal graded ideal, $reg(Sym_R(I))$. In general the problem is hard, but if I is generated by an s-sequence, our approach gives some interesting results. We recall some results obtained about ideals generated by linear forms as relation ideals of special symmetric algebras and we consider some basic properties about $s-$sequences and, additionally, we recall how to compute the invariants ([3], [4])and then we find sufficient and necessary conditions so that they are generated by $s-$sequences ([5]).

References

[1] Avramov, L.L. 1981 *Complete intersections and symmetric algebras*. Journal of Algebra 73, pp. 248–263.

[2] Herzog, J. Restuccia G. and Tang Z. 2001 *s-Sequences and symmetric algebras*. Manuscripta Math. 104, 479–501.

[3] Restuccia, G. 2006 *Symmetric algebras of finitely generated graded modules and s-sequences*. Rend. Sem. Mat., Univ. Pol. Torino 64(4), 479-496.

[4] Restuccia, G. 1986 *Formes linéaires et algèbres symétriques*. Bull. Sc. Math. II (110), 391-410.

[5] Restuccia, G and Staglianò, P.L. 2015 *Ideals generated by linear forms and symmetric algebras*. Ann. Acad. Rom. Sci. Ser. Math. Appl. 7 (2), 260–270.

On the 3-th hypersimplex and applications

Anna Maria Stanganelli
Dipartimento di Scienze Matematiche, Informatiche, Scienze Fisiche e Scienze della Terra
Viale Ferdinando D'Alcontres, 31, 98166 MESSINA
stanganelliannamaria@gmail.com

We define r-th hypersimplex A_r as the set of lattices points of N^n, N the semigroup of natural number, whose coordinates are $(i_1, i_2, ..., i_n)$, with $i_1 + i_2 + ... + i_n = r$, and $i_t \in \{0, 1\}$. For $r = 2$, the 2-nd hypersimplex A_2 is studied in [2], where one proved that the Groebner basis of the toric ideal I_{A_2}, with respect to the lexicographic order coincides with the Groebner basis with respect to the reverse lexicographic order and to the sorted order. All bases consist of binomials of degree two and the bases are the same. For $r = 3$, the situation is different. The sorted Groebner basis of the toric ideal I_{A_3} consists of binomials of degree two, but both lexicographic and reverse lexicographic Groebner basis are not quadratic. Since the most popular term orders are doubless the lex or the reverse lexicographic orders, we are interested to establish lower and upper bounds for the degree of these basis, since the triangulations associated can be more interesting in different fields, in particular from the geometric point of view. Some results contained in [2], where a sorted quadratic Groebner bases is found for the 3-th Veronese algebra, subalgebra of the polynomial ring $K[x_1, ..., x_n]$ in n variables on the field K (supposed algebraic closed) generated on K by all monomials of degree 3 in $x_1, ..., x_n$, can be revisited looking to find a quadratic sorted Groebner basis for the 3-th squarefree Veronese algebra, subalgebra of $K[x_1, ..., x_n]$, generated on K by all squarefree monomials of degree 3 in $x_1, ..., x_n$ by the application of the elimination theory, used in Groebner basis theory. Now, A_2 describes the algebra associated to a simple complete graph G_2 and A_3 describes the graph G_3 of paths of lenght 2 in the graph G_2. From this fact the importance of these problems arise in combinatorics and in many fields. For a low number of variables the problem is investigated and some interpretations in graph theory are given.

References

[1] A. Stanganelli, On the r-th hypersimplex and applications, preprint 2016.

[2] B. Sturmfels, Groebner bases and convex polytopes, Univ. Lect. Series, Vol. 8, Amer. Math. 1995.

Necessary data for some evaluation codes in the 2-dimensional case

Maurizio Imbesi
Università degli Studi di Messina
Viale F. Stagno d'Alcontres, 31 98166 - Messina Italy
imbesim@unime.it

Mustapha Lahyane
Universidad Michoacana de San Nicolás de Hidalgo
Avenida Francisco J. Múgica s/n 58040 - Morelia Mexico
lahyane@ifm.umich.mx

Jesús Adrián Cerda-Rodríguez
Universidad Politécnica de Aguascalientes
Calle Paseo San Gerardo, 207 Fracc. San Gerardo 20342 - Aguascalientes Mexico
jesus.cerda@upa.edu.mx

Nowadays, the urgent need to achieve, as soon as possible, the globalization in our planet requires the security of all data transfers from one source to another. In particular, it is very deseable to have evaluation codes with very good parameters.

It seems that smooth projective varieties offer concretely such codes, see for example [3] in the one-dimensional case, and [1, 2] in the two-dimensional case.

The aim of our study is to compute the dimensions of some families of evaluation codes which are constructed from the geometry of some smooth projective rational surfaces, see [4].

Let X_n^r be the smooth projective rational surface obtained as the blowing-up of the Hirzebruch surface Σ_n at the zero-dimensional closed subscheme $\bigcup_{i=1}^r \{P_i, Q_i\}$, where n and r are positive integers, and $\bigcup_{i=1}^r \{P_i, Q_i\}$ is a suitable set of points in Σ_n. Then it holds:

Theorem. *With the above notation, if n and r are such that the integer $n^2+2(2-r)n+4$ is positive, then the dimension of global sections of any invertible sheaf on X_n^r is computed.*

Our original interests of handling these kinds of codes are mainly their use in cryptography and as an instrument for the benefit of humanity.

In fact regarding cryptography, they can be considered as a way not only to encrypt data but also to authenticate users. And regarding the benefit of humanity, they can be implemented in Radio-Frequency Identification (RFID). The latter (with the help of a chip) enables from any place to identify, follow, get medical history and commercial tendencies of any human and can be used also as a tool of payment, to mention a few gentle applications.

References

[1] Davis, J.A. 2011 *Algebraic geometric codes on anticanonical surfaces.* J. Pure Appl. Algebra 215, 4, 496–510.

[2] Galindo, C. and Monserrat, F. 2009 *δ-sequences and evaluation codes defined by plane valuations at infinity.* Proc. Lond. Math. Soc. 98, 3, 714–740.

[3] Goppa, V.D. 1984 *Codes and information.* Uspekhi Mat. Nauk 39, 1, 77–120.

[4] Mumford, D. 1966 *Lectures on curves on an algebraic surface*. Ann. Math. Studies, vol. 59, Princeton Univ. Press.

The role of symmetry for the computation of nonlinear eigenvalues related to the electromagnetic parameters of microwave structures

Mario Versaci
DICEAM, Universitá *Mediterranea* di Reggio Calabria
via Graziella - Loc. Feo di Vito, 89121 - Reggio Calabria Italy
mario.versaci@unirc.it

Giovanni Angiulli
DIIES, Universitá *Mediterranea* di Reggio Calabria
via Graziella - Loc. Feo di Vito, 89121 - Reggio Calabria Italy
giovanni.angiulli@unirc.it

The numerical evaluation of parameters having practical interest in microwave engineering (e.g., cutoff wavenumbers or resonant frequencies of resonant structures) is often closely linked to the computation of a set of nonlinear eigenvalues, for which the related nonlinear eigenproblem $L(\gamma)f = 0$, with $\gamma \in \Omega \subset \mathbb{R}^+$ admits a non trivial solution [2]. This set is usually evaluated, after to have obtained a matrix representation $\mathbf{L}(\gamma)$ of the operator $L(\gamma)$ by a projective method, through the use of the Singular Value Decomposition. However this approach has a main drawback that is very time consuming due to its asymptotic computational cost of $\mathcal{O}(n^3)$ (where n is the order of $\mathbf{L}(\gamma)$). In [1] was developed a fast algorithm for computing this set of nonlinear eigenvalues. It is possible to empower the approach described in [1], exploiting the symmetry of the domain D on which is defined the nonlinear eigenproblem. In fact, collecting all the symmetry operations on D in a group $\mathcal{G}$ and building $\forall\tau \in \mathcal{G}$ a suitable matrix representation $\{\mathbf{M}(\tau)\}$, Group Theory states by means of the Shur's lemma [3] that this may always be decomposed into a direct sum of irriducible representations, i.e. exists a similarity transformation $\mathbf{S}$ such that $\mathbf{SM}(\tau)\mathbf{S}^{-1} = \mathbf{M}^{\beta}(\tau)$, where $\mathbf{M}^{\beta}(\tau)$ will have a block diagonal form $\forall\tau \in \mathcal{G}$. If the same basis representation is used to obtain $\mathbf{L}(\gamma)$ and if $\mathbf{L}(\gamma)$ commutes with $\mathbf{M}(\tau)$ for all $\tau \in \mathcal{G}$ (and this is the case for many nonlinear eigenproblem related to microwave problems) it is straightforward to demonstrate that relatively to the same symmetrizing basis described by the linear transformation $\mathbf{S}$, the matrix operator $\mathbf{L}(\gamma)$ will have a block diagonal form $\mathbf{L}^{\beta}(\gamma)$. This block diagonal representation for the original matrix problems will allow to solve, applying the method described in [1], a number p of reduced order decoupled nonlinear eigenproblem, obtaining in this way a very notable computational saving having order $\mathcal{O}((n/p)^3)$ where p is the number of irriducible blocks of $\mathbf{L}^{\beta}(\tau)$.

References

[1] Angiulli, G. 2007 *On the Computation of Nonlinear Eigenvalues in Electromagnetic Problems*, J. of Electr. Waves and Applications, vol.21, no.4, pp.527-532.

[2] Hanson, G. Yakovlev, A. B. 2001 *Operator Theory for Electromagnetics*, Springer-Verlag.

[3] Inui, T. Tanabe Y., Onodera, Y. 1990 *Group Theory and Its Applications in Physics*. Springer-Verlag.

Advances in Regularization Methods for Applied Inverse Problems

PROPOSERS

Germana Landi
Università degli Studi di Bologna
piazza Porta S. Donato, 5 40127 - Bologna Italy
germana.landi@unibo.it

Marco Prato
Università degli Studi di Modena e Reggio Emilia
via Campi, 213/b 41125 - Modena Italy
marco.prato@unimore.it

SPEAKERS

Alessandro Benfenati
CNRS, Université de Paris-Est Marne-la-Vallée
bnflsn@unife.it

Valentina De Simone
Dip. Matematica e Fisica, Seconda Università di Napoli
valentina.desimone@unina2.it

Marco Donatelli
Dip. Scienza e Alta Tecnologia, Università dell'Insubria
marco.donatelli@uninsubria.it

Silvia Gazzola
Sch. Engineering and Physical Sciences, Heriot-Watt University
sg39@hw.ac.uk

Alberto Sorrentino
Dip. Matematica, Università di Genova
sorrentino@dima.unige.it

Fabiana Zama
Dip. Matematica, Università di Bologna
fabiana.zama@unibo.it

The inverse problems theory has been investigated extensively in the past few decades due to its importance in several applications, the availability of new generations of computers and the development of reliable numerical methods. Applications such as image deconvolution and reconstruction and machine learning are examples that, combined with the large amount of data to be processed (think of 3D images or problems of automatic categorization of web pages), require powerful computers and appropriate numerical strategies in order to obtain an effective solution possibly in real time.
Inverse problems, posed as mathematical models of real physical phenomena, are a

multidisciplinary scientific field involving physics, engineering and different branches of mathematics. Regularization techniques are necessary to stabilize inverse problems, ill-posed by their nature. Recent advances in the numerical solution of inverse problems exploit the relationship between regularization methods and linear algebra and optimization algorithms. Many methods for solving inverse problems use classical linear algebra and numerical optimization algorithms and, at the same time, new strategies in linear algebra and numerical optimization have been recently developed starting from specific features of the inverse problems, such as their typical ill-posedness in the sense of Hadamard.
Objective of this symposium will be the presentation of recent numerical methods inspired by, or applied to, regularized models arising in specific inverse problems in astronomy, microscopy, finance or medicine.

Scaling Techniques for ε–subgradients methods

Alessandro Benfenati
Université Paris–Est, LIGM (UMR 8049), CNRS, ENPC, ESIEE Paris, UPEM
5 bd Descartes, Champs-sur-Marne, 77454 - Marne-la-Vallée, France
alessandro.benfenati@esiee.fr

Silvia Bonettini
Dipartimento di Matematica ed Informatica, Università di Ferrara, Polo Scientifico Tecnologico
Via Giuseppe Saragat 1, 44122 - Ferrara Italy
silvia.bonettini@unife.it

Valeria Ruggiero
Dipartimento di Matematica ed Informatica, Università di Ferrara, Polo Scientifico Tecnologico
Via Giuseppe Saragat 1, 44122 - Ferrara Italy
valeria.ruggiero@unife.it

Several models arising in relevant applications such as image and signal restoration, statistical inference and data analysis lead to the following constrained optimization problem

$$\min_{x\in\mathbb{R}^n} f(x) + \Phi(x) \tag{1}$$

where $f, \Phi : \mathbb{R}^n \to \mathbb{R} \cup \{\infty\}$ are convex, proper, lower semicontinuous functions and $\mathrm{dom}(\Phi) \subset \mathrm{dom}(f)$. Let denote with X^* the set of solutions of (1) and let $f^* = \inf_{x\in\mathbb{R}^n} f(x) + \Phi(x)$. We propose the following scaled forward–backward ε_k–subgradient scheme:

$$x^{(k+1)} = \mathrm{prox}_{\alpha_k\Phi, D_k^{-1}}\left(x^{(k)} - \alpha_k D_k u^{(k)}\right) \tag{2}$$

where D_k is a symmetric positive definite matrix with bounded eigenvalues, $u^{(k)} \in \partial_{\varepsilon_k} f(x^{(k)})$ for $\varepsilon_k \geq 0$ and α_k can be chosen either as an *a priori* selected sequence obeying to the Ermoliev rule $(\mathcal{R}_1)$ or with an adaptive rule $(\mathcal{R}_2)$ of Brännlund's type [4].

$(\mathcal{R}_1)$ $\alpha_k > 0, \lim_{k\to\infty} \alpha_k = 0, \sum \alpha_k = \infty, \sum \alpha_k^2 < \infty$

$(\mathcal{R}_2)$ $\alpha_k = \frac{f(x^{(k)}) - f_k}{\|u^{(k)}\|^2}$ or $\alpha_k = \frac{f(x^{(k)}) - f_k}{\max\{1, \|u^{(k)}\|^2\}}$

We provide a convergence analysis of the iteration (2) under suitable assumptions on sequences $\{u_k\}$ and $\{\epsilon_k\}$, the subgradient of Φ and different choices α_k. A convergence rate estimate can be obtained for α_k as in $\mathcal{R}_1$. Borrowing ideas of [5], we develop a Scaled forward–backward ε-Subgradient Level Algorithm (SSL) for a practical implementation of $\mathcal{R}_2$: details can be found in [2].
A concrete example of the method (2) can be devised for the problem

$$\min_{x\in\mathbb{R}^n} f_0(x) + f_1(Ax) + \Phi(x), \tag{3}$$

where $A \in \mathbb{R}^{m\times n}$, $f_0(x), f_1(x), \Phi(x)$ are convex, proper, lower semicontinuous functions such that $\mathrm{diam}(\mathrm{dom}(f_1^*))$ is finite and $f_1^*(y)$ is the Fenchel dual of f_1. Clearly, (3) is a

special case of (1). For the solution of (3), we propose the following Scaled Primal–Dual Hybrid Gradient (SPDHG) method for the solution of (3)

$$y^{(k+1)} = \text{prox}_{\tau_k f_1^*, I}(y^{(k)} + \tau_k A x^{(k)}) \quad (4)$$

$$u^{(k)} = d^{(k)} + A^T y^{(k+1)} \quad (5)$$

$$x^{(k+1)} = \text{prox}_{\alpha_k \Phi, D_k^{-1}}(x^{(k)} - \alpha_k D_k u^{(k)}) \quad (6)$$

where $d^{(k)} \in \partial_{\mu_k} f_0(x^{(k)})$, for some $\mu_k \geq 0$, and $\{\tau_k\}$, $\{\alpha_k\}$ are the dual and primal steplength sequences respectively. Method (4)–(6) is a special case of (2), where $f = f_0 + f_1 \circ A$. $A^T y^{(k+1)}$ is an ε-subgradient of $f_1 \circ A$ at $x^{(k)}$, as stated in [3, Lemma 1]: thus, $u^{(k)} = d^{(k)} + A^T y^{(k+1)} \in \partial_{\varepsilon_k} f(x^{(k)}), \varepsilon_k = \mu_k + \psi_k$. We provide two different SPDHG implementations, depending on the choice for the sequences.

Prefixed sequences. Let $\{\tau_k\}$, $\{\alpha_k\}$, $\{\gamma_k\}$ be sequences chosen a–priori, such that $\alpha_k = \mathcal{O}\left(k^{-p}\right), \tau_k = \mathcal{O}(k^p), \gamma_k = \mathcal{O}\left(k^{-q}\right), \frac{1}{2} < p \leq 1, q > 1$; define $L_k = \max\{\|D_k\|, \|D_k\|^{-1}\}$ and assume $L_k \leq \sqrt{1+\gamma_k}$ and μ_k convergent to zero at least as $\frac{1}{\tau_k}$. Then $\liminf_{k\to 0} f(x^{(k)}) + \Phi(x^{(k)}) = f^*$; if $X^* \neq \emptyset$, the sequence $\{x^{(k)}\}$ converges to a solution of (3) and $\lim_{k\to\infty} f(x^{(k)}) + \Phi(x^{(k)}) = f^*$

Adaptive primal sequence. Let $\{x^{(k)}\}$ be the sequence generated by SSL Algorithm, $\lim_{k\to\infty} \tau_k = \infty$, $\gamma_k = \mathcal{O}\left(k^{-q}\right)$ then we have $\liminf_{k\to\infty} f(x^{(k)}) + \Phi(x^{(k)}) = f^*$.

We further specialize the SPDHG method for a specific application in the image restoration context: let $f_0(x) \equiv f_0(Hx + b; g)$ be the Kullback–Leibler functional, where $g \in \mathbb{R}^n$ is a detected image, corrupted by Poisson noise, $H \in \mathbb{R}^{n\times n}$ represents the blurring operator (with standard assumptions) while $b \in \mathbb{R}$ is a nonnegative background term. The regularization term is given by $f_1(Ax) = \beta TV(x)$, $\beta > 0$, i.e. the Discrete Total Variation functional. The function $\Phi(x)$ is the indicator function of the set $X = \{x \in \mathbb{R}^n : x_i \geq 0\}$. In order to devise a suitable scaling matrix D_k for SPDHG, we adapt to our case the split gradient strategy proposed in [1] for nonnegatively constrained differentiable problems. We consider four different versions of the method (4)–(6) to solve the problem (3) in the image restoration framework:

PDHG corresponds to set $D_k = I$ and α_k satisfying $\mathcal{R}_1$. It consists in the method in [3];

SPDHG α_k is chosen such that it satisfies $\mathcal{R}_1$;

SL is the SSL procedure with $D_k = I$ and $u^{(k)} = \nabla f_0(x^{(k)}) + \beta A^T y^{(k+1)}$, where $y^{(k+1)}$ is updated as in (4);

SSL is the same as above but with the scaling matrix D_k defined as in SPDHG.

From the numerical experience we observe that the presence of the scaling can help to accelerate the progress towards the solution, with both stepsize selection strategies. As concerns the scaling matrix bounds, the best results are obtained by selecting large initial values for γ_k, allowing more freedom to choose D_k. It is also interesting to observe that the adaptive computation of α_k combined with the proposed scaling technique in SSL seems to work quite well, leading to performances that are, in some cases, close to the 'best' ones obtainable by manually tuning the stepsize sequence in PDHG and SPDHG.

References

[1] Bertero, M. and Lanteri, H. and Zanni L. 2008, Iterative image reconstruction: a point of view. In *Mathematical Methods in Biomedical Imaging and Intensity-Modulated Radiation Therapy (IMRT)* pages 37–63.

[2] Bonettini, S. and Benfenati, A. and Ruggiero, V. 2016, Scaling Techniques fo ε–Subgradient Methods. In *arXiv:1407.6133v2 [math.NA]*, under revision.

[3] Bonettini, S. and Ruggiero, V. 2012, On the convergence of primal-dual hybrid gradient algorithms for total variation image restoration. In *J. Math. Imaging Vis.*, vol. 44, pages 236–253.

[4] Brännlund, U. and Kiwiel, K.C. and Lindberg P.O. 1995, A descent proximal level bundle method for convex nondifferentiable optimization. In *Oper. Res. Lett.*, vol. 17, pages 121–126.

[5] Goffin, J.L. and Kiwiel, K.C. 1999, Convergence of a simple subgradient level method. In *Mathematical Programming*,vol. 85, pages 207–211.

An iterative regularization method for portfolio selection

Valentina De Simone
Seconda Università degli Studi di Napoli
viale Lincoln, 5 81100 - Caserta Italy
valentina.desimone@unina2.it

Stefania Corsaro
Università degli Studi di Napoli "Parthenope"
Via Generale Parisi, 13 80132 - Napoli Italy
stefania.corsaro@uniparthenope.it

We consider the problem of portfolio selection within the classical Markowitz mean-variance framework [3]. Given n traded assets, the problem is to establish the amount of capital to be invested in each one of them to build an investment portfolio with minimum risk for a fixed expected return. We assume that one unit of capital is available and denote with $\mathbf{w} = (w_i)_{i=1,n}$ the portfolio weight vector, that is, the amount w_i is invested in the $i-th$ asset. Let $\mu = (\mu_i)_{i=1,n}$ where μ_i is the expected return of asset i, and $\mathbf{t}$ a set of m evenly spaced dates at which asset returns are estimated, so that r_{ti} is the return of asset i at time t. If one estimates expectations by means of sample averages, portfolio selection is formulated in the following form:

$$\begin{array}{l} \min_{\mathbf{w}} \frac{\mathbf{1}}{m}\|\rho 1_m - R\mathbf{w}\|_2^2 \\ \text{s.t.} \\ \mathbf{w}^T\mu = \rho \\ \mathbf{w}^T\mathbf{1}_n = 1, \end{array} \tag{1}$$

where R is the $m \times n$ matrix containing asset returns, ρ is the fixed expected portfolio return and $\mathbf{1}_l$ is the unitary vector of length l. In (1) the first constraint fixes the expected return and the second one is a budget constraint which establishes that all the available capital is invested. If asset returns are highly correlated, then R is ill-conditioned. Different regularizations have been proposed, we focus on the following regularized problem [2]:

$$\begin{array}{l} \min_{\mathbf{w}} \|\rho\mathbf{1}_m - R\mathbf{w}\|_2^2 + \tau\|\mathbf{w}\|_1 \\ \text{s.t.} \\ \mathbf{w}^T\mu = \rho \\ \mathbf{w}^T\mathbf{1}_n = 1 \end{array} \tag{2}$$

in which the l_1 penalty term provides sparse solutions.
In this talk we discuss an iterative regularization method for problem (2), based on Bregman approach [1] with an adaptative rule for the estimation of τ that avoids negative weights corresponding to undesired *short sales*. Numerical experiments on real market data are presented to show the effectiveness of our strategy.

References

[1] Bregman, L. 1967 *The relaxation method of finding the common points of convex sets and its application to the solution of the problems in convex optimization.* USSR Comput. Math. and Math. Physics 7, 200-217.

[2] Brodie, J., Daubechies, I., De Mol, C., Giannone, D. and Loris, I. 2009 *Sparse and stable Markowitz portfolios.* PNAS 106(30), 12267–12272.

[3] Markowitz, H. 1952 *Portfolio Selection.* The Journal of Finance 7(1), 77-91.

[4] Wotao,Y., Osher, S., Goldfarb, D. and Darbon, J. 2008 *Bregman Iterative Algorithms for l_1-Minimization with Applications to Compress Sensing.* SIAM J. Imaging Sciences 1(1), 143–168.

Regularization preconditioners for frame-based image deblurring

Marco Donatelli
Università degli Studi dell'Insubria
via Valleggio, 11 22100 - Como Italy
marco.donatelli@uninsubria.it

Davide Bianchi
Università degli Studi dell'Insubria
via Valleggio, 11 22100 - Como Italy
d.bianchi9@uninsubria.it

Yuantao Cai
University of Electronic Science and Technology of China
Chengdu, Sichuan, 611731, PR China
yuantaocai@163.com

Ting-Zhu Huang
University of Electronic Science and Technology of China
Chengdu, Sichuan, 611731, PR China
tingzhuhuang@126.com

Thresholding iterative methods have recently been successfully applied to image deblurring problems. In this talk, we investigate the modified linearized Bregman algorithm (MLBA) used in image deblurring problems [2], with a correct treatment of the boundary artifacts (see [4]). The fast convergence of the MLBA depends on a regularizing preconditioner that could be computationally expensive and hence it is usually chosen as a block circulant circulant block (BCCB) matrix, diagonalized by discrete Fourier transform.
We show that the standard approach based on the BCCB preconditioner may provide low quality restored images and we propose different preconditioning strategies, that enhance the quality of the restoration and save some computational cost at the same time. Motivated by a recent nonstationary preconditioned iteration introduced in [3] for least-square inverse problems, we propose a new algorithm that combines such method with the MLBA [1]. We prove that it is a regularizing and convergent method. A variant with a stationary preconditioner is also considered and some numerical results are compared with similar methods.

References

[1] Cai, Y. Donatelli, M. Bianchi, D. and Huang, T. Z. 2016 *Regularization preconditioners for frame-based image deblurring with reduced boundary artifacts*, SIAM J. Sci. Comput., 38–1, B164–B189.

[2] Cai, J. F. Osher, S. and Shen, Z. 2009 *Linearized Bregman iterations for frame-based image deblurring*, SIAM J. Imaging Sci., 2–1, 226–252.

[3] Donatelli, M. and Hanke, M. 2013 *Fast nonstationary preconditioned iterative methods for ill-posed problems, with application to image deblurring*, Inverse Problems, 29, 095008.

[4] Donatelli, M. and Serra-Capizzano, S. 2010 *Antireflective Boundary Conditions for Deblurring Problems*, Journal of Electrical and Computer Engineering, 2010, Article ID 241467.

Enforcing nonnegativity by flexible Krylov subspaces

Silvia Gazzola
University of Bath
Department of Mathematical Sciences, Bath BA2 7AY, United Kingdom
s.gazzola@bath.ac.uk

Constrained linear least squares problems arise in a variety of applications, and many iterative methods are already available to compute their solutions (cf., for instance, [1, 2] and the references therein).

This talk will introduce a new efficient approach (dubbed "MFCGLS") to solve nonnegative linear least squares problems

$$\min_{x \geq 0} \|b - Ax\|_2 \,. \qquad (*)$$

The main idea underlying MFCGLS is to leverage the KKT conditions in order to form an adaptively preconditioned unconstrained least squares problem, which is then solved by a flexible Krylov subspace method. Some properties of MFCGLS will be discussed, and some insight will be given.

The new method can be easily applied to image deblurring and denoising problems,

$$Ax^{ex} + n = b \,,$$

where the goal is to compute a good approximation of a sharp image x^{ex}, given a corrupted version b of it and a linear blurring model A. When dealing with images, nonnegativity is a very meaningful constraint to impose, since the entries of x^{ex} (pixels) represent nonnegative intensities.

The results of many numerical experiments will be displayed during the talk. When compared to many state-of-the-art solvers for nonnegative least squares, MFCGLS delivers results of equal or better quality, with a significant speedup. In this abstract, only a sample of these tests is proposed. Besides MFCGLS, the following well-known solvers are taken into account:

- FISTA [1]: in the special case of nonnegativity constraints, FISTA is an accelerated version of the projected gradient method.
- MRNSD [2]: this method can be regarded as a modified steepest descent approach applied to solve the adaptively preconditioned system stemming from the KKT conditions.
- CGLS (see [3]): the conjugate gradient method applied to the normal equations, in order to solve the unconstrained least squares problem associated to $(*)$.

Figure 1 displays the exact `galaxy` image, a blurred and noisy version of it, and the best reconstructions obtained by different method. Table 1 reports the best attained relative error (i.e., $\|x^{ex} - x_m\|_2 / \|x^{ex}\|_2$), the corresponding iteration m, and the average time per iteration. Finally, Figure 2 displays the history of the relative errors for the considered methods. Looking at these results, one can see that considering nonnegativity constraints

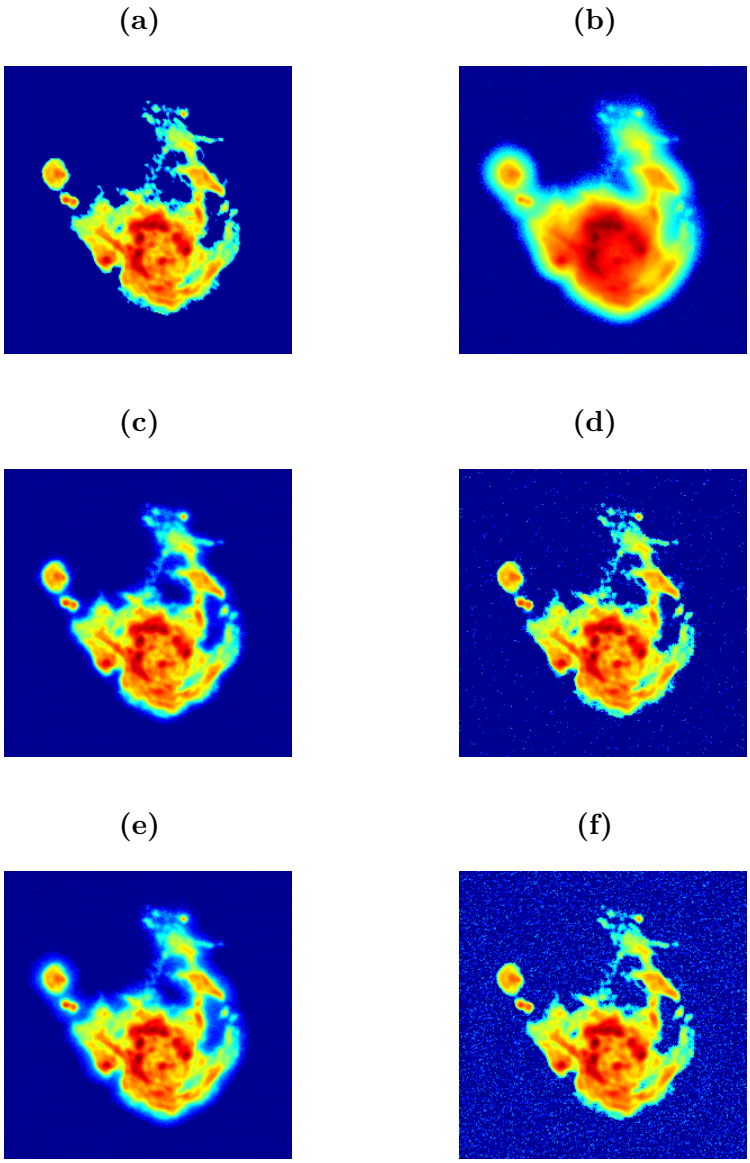


Figure 1: `galaxy` images in logarithmic scale. **(a)** exact. **(b)** blurred and noisy. **(c)** reconstruction by MFCGLS. **(d)** reconstruction by FISTA. **(e)** reconstruction by MRNSD. **(f)** reconstruction by CGLS.

	rel.error	**iterations**	**av.time**
MFCGLS	0.0351	26	0.37
FISTA	0.0311	58	0.61
MRNSD	0.0374	100	0.29
CGLS	0.0404	11	0.30

Table 1: Performance of the different methods employed to restore the `galaxy` test image.

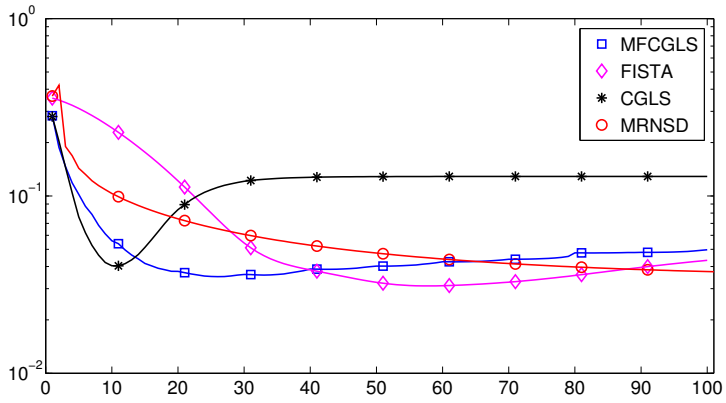


Figure 2: Relative errors versus the number of iterations for the different solvers employed to restore the `galaxy` test image.

enhances the quality reconstruction: indeed, the relative error of CGLS is much higher than the other methods. Note also that one iteration of each solver approximately has the same computational cost (which is dominated by two matrix-vector products, one with A and one with A^T). Since FISTA with backtracking is considered, more sub-iterations might be necessary at each iteration. In this framework, MFCGLS is very efficient, since it requires much fewer iterations to reach reconstructions of the same quality. The so-called semi-conference phenomenon clearly happens for all the methods except for MRNSD.

References

[1] Beck, A. and Teboulle, M. 2009, *A Fast Iterative Shrinkage-Thresholding Algorithm for Linear Inverse Problems*. SIAM Journal on Imaging Sciences 2(1), 183–202.

[2] Nagy, J. G. and Strakos, Z. 2000, Enforcing nonnegativity in image reconstruction algorithms. In *International Symposium on Optical Science and Technology*, pp. 182–190. International Society for Optics and Photonics.

[3] Saad, Y. 2003, *Iterative Methods for Sparse Linear Systems*. SIAM.

Iterative Algorithms for the Non–Linear LIDAR Inverse Problem

Alberto Sorrentino
Università degli Studi di Genova
sorrentino@dima.unige.it

Giulia Denevi
Università degli Studi di Genova
giulia.denevi@gmail.com

Sara Garbarino
University College London
s.garbarino@ucl.ac.uk

Michele Piana
Università degli Studi di Genova
piana@dima.unige.it

LIDARs are powerful imaging tools that illuminate a target object with a laser and then measure the reflected light. In the atmospheric application of LIDAR [1], the illuminated object is the atmospheric aerosol, that partially absorbs, partially transmits and partially reflects light, allowing to investigate its distribution up to several thousand meters. The (exact) measured signal $P(z)$ from height z is given by

$$P(z) = C\frac{\beta(z)}{z^2}\exp\left(-\int_0^z \alpha(z')dz'\right) \tag{1}$$

where C is a known constant, $\beta(z)$ is the backscattering coefficient and $\alpha(z)$ is the absorption coefficient. In Raman LIDAR, the backscattering coefficient is known, and only $\alpha(z)$ has to be recovered from noisy recordings of $P(z)$.
As the data are basically photon counts, it is natural to assume that noise is Poisson. In order to take this into account properly, one needs to solve the non–linear inverse problem described by (1); the simpler alternative (taking the logarithm of all known quantities and thus linearize the problem, such as in [2]) is not feasible, as the logarithm modifies the noise distribution.
We have devised three iterative algorithms for retrieving the absorption coefficient: two of them are Maximum Likelihood algorithms that need to be stopped early in order to achieve regularization; the third one contains an explicit L^2 regularization term that encourages smooth solutions. Two algorithms (one ML and one regularized) have been obtained as fixed–point algorithms from the Karush–Kuhn–Tucker conditions [3]; the other one is an Expectation–Maximization algorithm [4] with an approximated M–step as in [5]. In this talk we discuss the convergence properties of the algorithms and their relationship with current literature, and show applications to experimental LIDAR data.

References

[1] A. Ansmann, M. Riebesell and C. Weitkamp. *Measurement of atmospheric aerosol extinction profiles with a Raman lidar.* Opt. Lett., 15 (13), 746-748, 1990.

[2] P. Pornsawad, G. D'Amico, C. Boeckmann, A. Amodeo and G. Pappalardo. *Retrieval of aerosol extinction coefficient profiles from Raman lidar data by inversion method.* Opt. Lett., 51 (12), 2035-2044, 2012.

[3] H. Lantéri, M. Roche and C. Aime. *Penalized maximum likelihood image restoration with positivity constraints: multiplicative algorithms.* Inverse Problems, 18, 1397-1419, 2002.

[4] A. Dempster, N. M. Laird, and D. B. Rubin. *Maximum likelihood from incomplete data via the EM algorithm.* J. Roy. Statist. Soc., ser. B, 39, 1-38, 1977.

[5] K. Lange and R. Carson. *EM reconstruction algorithms for emission and transmission tomography.* J. Comput. Assist. Tomog., 8, 306-316, 1984.

Improved Inversion of two-dimensional NMR Relaxation data with the UPEN principle

Fabiana Zama
Dipartimento di Matematica, Università degli Studi di Bologna
Piazza di Porta San Donato, 5 40127, Bologna - Italia
fabiana.zama@unibo.it

Villiam Bortolotti
Dipartimento di Ingegneria Civile, Ambientale e dei Materiali, Università degli Studi di Bologna
Viale Risorgimento, 2 - 40136, Bologna - Italia
villiam.bortolotti@unibo.it

Robert Brown
Pomona CA 91767-2024 - USA
rjsbmeb@mailaps.org

Paola Fantazzini
Dipartimento di Fisica e Astronomia, Università degli Studi di Bologna
Viale Berti Pichat, 6/2 - 40127, Bologna - Italia
paola.fantazzini@unibo.it

Germana Landi
Dipartimento di Matematica, Università degli Studi di Bologna
Piazza di Porta San Donato, 5 40127, Bologna - Italia
germana.landi@unibo.it

Two-dimensional NMR relaxation data are commonly represented by a signal measured at different time sampling points (t_1,t_2) and their inversion requires the solution of the first-kind Fredholm integral equation:

$$S(t_1,t_2) = \iint_0^\infty k_1(t_1,T_1)k_2(t_2,T_2)F(T_1,T_2)\ dT_1\ dT_2 + e(t_1,t_2). \tag{1}$$

where the kernel is represented by the product of the functions $k_1(t_1,T_1) = 1-2\exp(-t_1/T_1)$, and $k_2(t_2,T_2) = \exp(-t_2/T_2)$. The function $e(t_1,t_2)$ represents additive noise, commonly modeled by a Gaussian distribution. Finally the unknown $F(T_1,T_2)$ is the distribution of longitudinal and transverse relaxation times.
Problem (1) is discretized by considering $M_1 \times M_2$ samples of the times t_1, t_2 and by organizing the discrete observations $\mathbf{S} \in \mathbb{R}^{M_1\times M_2}$ in a vector $\mathbf{s} \in \mathbb{R}^M$, $M = M_1 \times M_2$. The unknown discrete distribution $\mathbf{F} \in \mathbb{R}^{N_x\times N_y}$ is obtained by sampling F at $N_x \times N_y$ relaxation times T_1 and T_2 and it is organized in a vector $\mathbf{f} \in \mathbb{R}^N$, $N = N_x \times N_y$. Problem (1) is discretized as:

$$\mathbf{K}\mathbf{f} + \mathbf{e} = \mathbf{s} \tag{2}$$

where the matrix $\mathbf{K}$ is the Kronecker product

$$\mathbf{K} = \mathbf{K}_2 \otimes \mathbf{K}_1 \tag{3}$$

of the matrices $\mathbf{K}_1 \in \mathbb{R}^{M_1 \times N_x}$ and $\mathbf{K}_2 \in \mathbb{R}^{M_2 \times N_y}$ obtained by discretization of the functions k_1 and k_2 in $M_1 \times N_x$ and $M_2 \times N_y$ points respectively. The vector $\mathbf{e} \in \mathbb{R}^M$ is the discretization of the noise function $e(t_1, t_2)$.
In this talk we present the Improved 2DUPEN algorithm (I2DUPEN) that extends the Uniform Penalty (UPEN) algorithm [1] to two-dimensional data. The ill-conditioning of the linear model (2) is well known and Tikhonov regularization is commonly applied to the inversion of NMR data. It is well known that the main difficulty of the Tikhonov method is the estimation of the regularization parameter. Furthermore a single regularization parameter does not allow one to reconstruct peaks and flat regions with the same accuracy. For this reason, we consider multiple parameter Tikhonov regularization and we use the UPEN principle [1] as a suitable criterion for choosing the regularization parameters. In this context, given an initial guess $\mathbf{f}^{(0)}$, the local values of the regularization parameters and the corresponding approximate solution are obtained by means of the following iterative scheme [2].

Iterative scheme

Step 1 Compute $\lambda_i^{(k)}$ as follows

$$\lambda_i^{(k)} = \frac{\|\mathbf{K}\mathbf{f}^{(k)} - \mathbf{s}\|^2}{N\left(\beta_0 + \beta_p \max_{\mu \in I_i} (p_\mu^{(k)})^2 + \beta_c \max_{\mu \in I_i} (c_\mu^{(k)})^2\right)}, \quad i = 1, \ldots, N \tag{4}$$

Step 2 Compute $\mathbf{f}^{(k+1)}$ by solving

$$\min_f \ \|\mathbf{K}\mathbf{f} - \mathbf{s}\|_{\mathbf{B}}^2 + \sum_{i=1}^{N} \lambda_i^{(k)} (\mathbf{L}\mathbf{f})_i^2 \tag{5}$$

Step 3 Set $k = k + 1$.

In our notation, $\mathbf{B} \in \mathbb{R}^{M \times M}$ is a diagonal matrix of weights related to the statistics of the data, $\mathbf{L} \in \mathbb{R}^{N \times N}$ is the discrete Laplacian operator, c_μ are the elements of $\mathbf{L}\mathbf{f}$, p_μ are the reordered elements of $\|\nabla \mathbf{F}\|$, the I_i are the indices subsets related to the neighborhood of the pixel i and the β's are positive parameters. The parameter β_0 prevents division by zero and is a compliance floor, which should be small enough to prevent undersmoothing, and large enough to avoid oversmoothing. The optimum value of β_0, β_c and β_p can substantially change with the nature of the measured sample. Therefore, their general optimum value can be only evaluated on the basis of statistical evaluation. Moreover, the data can be compressed using Singular Value Decomposition of the kernel to reduce the computation cost.
We report the results obtained on real NMR data. A sample was prepared by filling a 10 mm external diameter glass NMR tube with 6 mm of egg yolk. The tube was sealed with Parafilm, and then at once measured. NMR measurements were performed at 25° by a homebuilt relaxometer based on a PC-NMR portable NMR console (Stelar, Mede, Italy) and a 0.47 T Joel electromagnet. The $T_1 - T_2$ maps obtained from the I2DUPEN inversion are shown in figure 1. Figure 2 shows, in log-scale, the regularization matrix $\mathbf{\Lambda}$. The results of our numerical experiments highlight the potential of the proposed method in reconstructing both peaks and flat regions with the same accuracy while automatically estimating the regularization parameters.

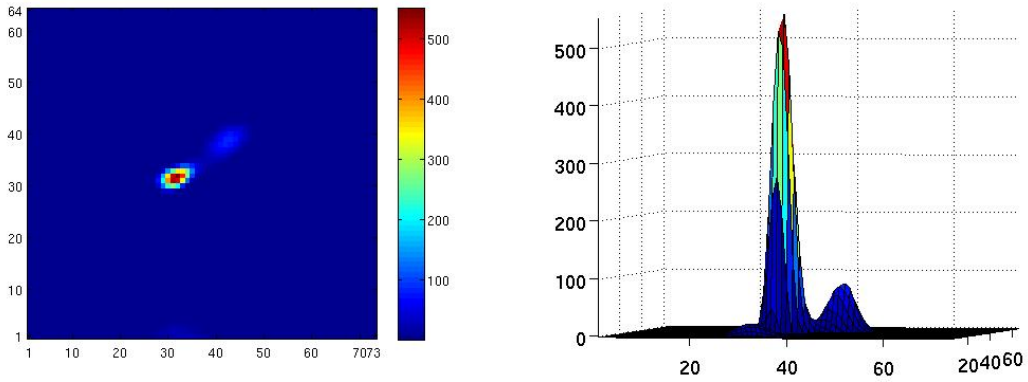


Figure 1: $T_1 - T_2$ maps (left) and 3D distributions (right), obtained by the I2DUPEN method.

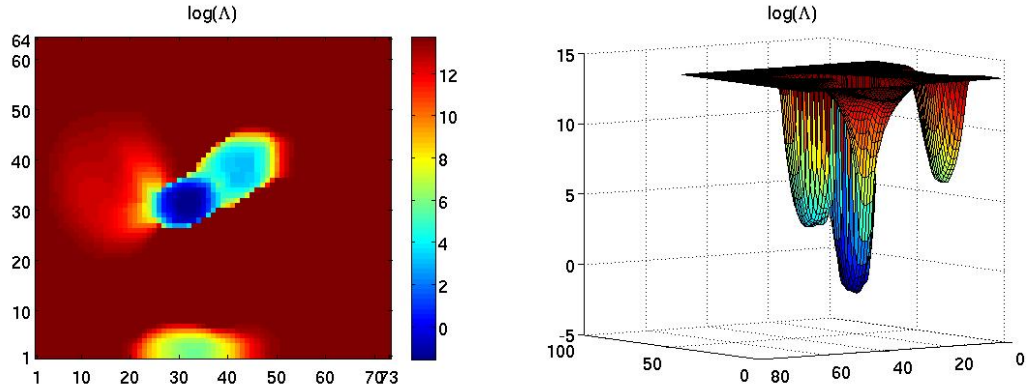


Figure 2: Regularization matrix $\log(\mathbf{\Lambda})$ of the I2DUPEN method.

References

[1] G.C. Borgia, R.J.S. Brown, and P. Fantazzini, *J. Magn. Res.*, 147(2):273-285,2000.

[2] V. Bortolotti, R.J.S. Brown, and P. Fantazzini G. Landi, F. Zama, submitted, 2016.

Dynamical Systems with discontinuities: theory, numerical methods and applications

PROPOSERS

Luciano Lopez
Università degli Studi di Bari
via E. Orabona, 5, 70125 - Bari Italy
luciano.lopez@uniba.it

Stefano Maset
Università degli Studi di Trieste
via Valerio 12/1 - 34127 - Trieste Italy
maset@units.it

SPEAKERS

Alessandro Colombo
Dept. of Electronics, Information and Bioengineering, Politecnico di Milano
alessandro.colombo@polimi.it

Raffaele D'Ambrosio
Dept. of Mathematics, University of Salerno
rdambrosio@unisa.it

Cinzia Elia
Dept. of Mathematics, Universitá di Bari
cinzia.elia@uniba.it

Bianca Giovanardi
MOX, Politecnico di Milano
bianca.giovanardi@polimi.it

Stefano Maset
Dept. of Mathematics and Geosciences, University of Trieste
maset@units.it

Luis Rández
Universidad de Zaragoza
randez@unizar.es

Discontinuous dynamical systems (DDSs) are often used to model problems arising in mechanics, control theory, economics, electrical engineering, chemistry reactions etc. (see [1]). The discontinuity can occur in the solution of the DDS, such as in impact problems, or in the derivative, such as in switching systems or Filippov systems. One of the main issues of DDS is that the derivative is not defined on some given discontinuity surfaces (see [2, 3]). This in turn raises questions such as whether the solution is unique on the discontinuity surfaces, how to regularize the discontinuous vector fields and how to build numerical schemes for discontinuous ODEs that retain a given accuracy. In

this minisymposium we will discuss the theoretical and numerical aspects of this class of dynamical systems such as their applications to PDEs.

References

[1] Acary, V. and Brogliato, B. 2008 *Numerical Methods for Nonsmooth Dynamical Systems. Applications in Mechanics and Electronics.* Lecture Notes in Applied and Computational Mechanics. Springer-Verlag, Berlin.

[2] Filippov, A. F. 1988 *Differential equations with discontinuous right hand sides*. Math. Appl. Kluwer Academic, Dordrechet.

[3] di Bernardo, M., Budd, C.J., Champneys, A.R. and Kowalczyk, P. 2008 *Piecewise-smooth Dynamical Systems: Theory and Applications*. Springer, Berlin..

Between smooth and piecewise smooth

Alessandro Colombo
DEIB, Politecnico di Milano
via Ponzio, 34/5 20133 - Milano Italy
alessandro.colombo@polimi.it

1 Smooth or piecewise smooth?

Piecewise smooth and slow-fast systems are frequently used as alternative mathematical representations of the same phenomenon. From an applied scientist's perspective, having a choice between two languages can be useful, for instance to pick the most appropriate formalism for a given numerical analysis tool, as long as the differences in the results that can be expected are well understood. Unfortunately, the differences in the behaviour of a smooth and piecewise smooth system that were built to be 'close' are rarely well understood.
This problem was addressed many times in the literature, and a fruitful branch of research started from the work in [3] on the smoothing of a two-dimensional piecewise smooth system. What we propose here is a small extension of this branch, mostly built on classical results available in [1]. Our main results can be roughly stated as follows:

Statement 1. *The dynamics of a piecewise smooth system is a superset of the dynamics of the smooth system it represents (i.e., of its smoothing).*

Statement 2. *The bifurcation diagram of a piecewise smooth system contains all transitions in the bifurcation diagram of its smoothing, but some of these transitions can take place simultaneously.*

These two statements are formalised in Theorems 1 and 2, respectively. With respect to existing results, they have the advantage of requiring no assumptions on dimensionality, the relative geometry of flow and discontinuity surfaces, or on structural stability. Furthermore, they are written assuming one smooth discontinuity boundary for the sake of simplicity, but nothing in the proof prevents their extension to arbitrarily many (possibly intersecting) boundaries. The next section simply collects definitions and lemmas from [1], reported here for reference. Our original results are in Section 3.

2 Preliminary results

Lemma 1 (Lemma 1 page 60 in [1])**.** *If two nonempty closed sets A and B do not have common points and B is bounded, then there exists points $a \in A$ and $b \in B$ such that* $\inf_{a\in A, b\in B} |a-b| = |a-b| > 0$.

Definition 1 (Upper semicontinuous)**.** *$F(\mathbf{x})$ is upper semicontinuous at the point $\mathbf{x}$ if*

$$\sup_{\dot{\mathbf{x}}'\in F(\mathbf{x}')} \inf_{\dot{\mathbf{x}}\in F(\mathbf{x})} \|\dot{\mathbf{x}}' - \dot{\mathbf{x}}\| \to 0 \text{ as } \mathbf{x}' \to \mathbf{x}.$$

(here $\|\cdot\|$ is the Euclidean norm.)

Definition 2 (Basic conditions)**.** *A set-valued function $F(t, \mathbf{x})$ in a domain G satisfies the basic conditions if, for all $(t, \mathbf{x}) \in G$, the set of $F(t, x)$ is nonempty, bounded, closed, convex, and the function F is upper semicontinuous in $t, \mathbf{x}$.*

Lemma 2 (Theorem 2 page 78 in [1])**.** *Let $F(t, \mathbf{x})$ satisfy the basic conditions in a closed bounded domain D. Then each solution of the inclusion $\dot{\mathbf{x}} \in F(t, \mathbf{x})$ lying within D can be continued on both sides up to the boundary of the domain.*

Definition 3. *A vector function $y(t)$ is a δ-solution of the inclusion $\dot{x} \in F(x, t)$ with F upper semicontinuous in t, x if on a given interval the function $y(t)$ is absolutely continuous and almost everywhere $\dot{y}(t) \in [coF(t^\delta, y^\delta)]^\delta$.*

Lemma 3 (Lemma 1 page 87 in [1])**.** *Let $F(t, x)$ satisfy the basic conditions in the open domain G, and let $\{\mathbf{x}_i(t)\}$ bet a sequence of δ_i-solutions of*

$$\dot{\mathbf{x}} \in F(t, x) \tag{1}$$

lying for $a_i \leq t \leq b_i$ in a closed and bounded domain G, with

$$\delta_i \to 0, \quad a_i \to a, \quad b_i \to b, \quad \mathbf{x}_i(a_i) \to x_0, \quad x_i(b_i) \to x^*.$$

Then, from the sequence $\{\mathbf{x}_i(t)\}$ one can extract a subsequence which converges uniformly to the solution $x(t)$ of (1) on each $[a', b'] \in [a, b]$, and $x(a) = x_0$, $x(b) = x^*$.

Lemma 4 (Theorem 3 page 79 in [1])**.** *Let the function $F(t, \mathbf{x})$ satisfy the basic conditions in the domain G. Let all solutions of $\dot{\mathbf{x}} \in F(t, \mathbf{x})$ exist for $a \leq t \leq b$ and their graphs lie in G. Then the set H of the points lying on these graphs at $a \leq t \leq b$ is bounded and closed.*

3 Main results

The following theorem proves that each orbit of the smoothing of a piecewise smooth system[2] uniformly converges to an orbit of the piecewise smooth system.

Theorem 1. *Consider the two systems Σ_1 and Σ_2 defined as follows*

$$\begin{aligned}
&\Sigma_1 : \\
&\quad \dot{\mathbf{x}} = F_1(t, \mathbf{x}) := f^+(\mathbf{x}, \mathbf{y})\phi(h(\mathbf{y})/\epsilon) + f^-(\mathbf{x}, \mathbf{y})(1 - \phi(h(\mathbf{y})/\epsilon)) \\
&\quad \phi(\cdot) \in [\lambda_l, \lambda_h] \\
&\quad \phi(h(\mathbf{y})/\epsilon) = 1 \text{ when } h(\mathbf{y})/\epsilon \geq 1 \\
&\quad \phi(h(\mathbf{y})/\epsilon) = -1 \text{ when } h(\mathbf{y})/\epsilon \leq -1,
\end{aligned}$$

and

$$\Sigma_2 : \qquad \dot{\mathbf{x}} \in F_2(t, \mathbf{x}) := \begin{cases} f^+(\mathbf{x}, \mathbf{y}), & h(\mathbf{y}) > 0 \\ f^-(\mathbf{x}, \mathbf{y}), & h(\mathbf{y}) < 0, \\ \text{co}\{\lambda_h f^+(\mathbf{x}, \mathbf{y}), \lambda_l f^+(\mathbf{x}, \mathbf{y}), & \\ \quad (1 - \lambda_h) f^-(\mathbf{x}, \mathbf{y}), (1 - \lambda_l) f^-(\mathbf{x}, \mathbf{y})\}, & h(\mathbf{y}) = 0. \end{cases}$$

[2] In fact, of a slight generalization of the smoothing in [3] where the smoothing function ϕ is allowed to take values in an arbitrary interval $[\lambda_l, \lambda_h]$, as long as it goes to ± 1 out of an ϵ-neighbourhood of the discontinuity

Solutions of Σ_2 are intended in the sense of Filippov. Assume that Σ_2 satisfies the basic conditions, and all its solutions exist for $a \le t \le b$ and have graph in an open domain G. Then, each orbit of Σ_1 uniformly converges to an orbit of Σ_2 in G for $\epsilon \to 0$.

Proof. By Lemma 4 the set H of points $(t, \mathbf{x})$, $a \le t \le b$, belonging to the graph of solutions of Σ_2 is closed and bounded. By Lemma 1

$$\inf_{\alpha \in H, \beta \in \partial G} |\alpha - \beta| = \rho_0 > 0. \tag{2}$$

Take a closed and bounded d-neighbourhood H^d of H, with $0 < 2d < \rho_0$, and take a sequence $x_i(t)$ of solutions of $\Sigma_1(\epsilon_i)$, $i = 1, 2, \ldots$, with $|t_{0i} - t_0| \le \epsilon_i, \quad |x_{0i} - x_0| \le \epsilon_i$. We have by construction that

$$F_1 \subset [\mathrm{co} F_2(t^{\epsilon_i}, x^{\epsilon_i})]^{\epsilon_i} \tag{3}$$

By (2) H^d is contained in G, so by Lemma 2 each solutions $x_i(t)$ can be continued both sides up to the boundary of H^d, and since H^d contains H, all $x_i(t)$ exist for all $t \in [a, b]$. Also observe that all solutions $x_i(t)$ are absolutely continuous, being integrals of F_1, therefore by (3) they are ϵ_i-solutions of Σ_2. By Lemma 3 a subsequence of $\{\mathbf{x}_i(t)\}$ converges uniformly to a solution of Σ_2. □

Definition 4 (from [2])**.** *Two families of dynamical systems $\Sigma_{1,\epsilon}(p)$ and $\Sigma_{1,\epsilon'}(p')$ in the parameter p are topologically equivalent if*

- *there exists a homeomorphism of the parameter space $h_{\epsilon,\epsilon'} : \mathbb{R} \to \mathbb{R}$, $p' = h_{\epsilon,\epsilon'}(p)$,*
- *there exists a parameter-dependent homeomorphism of the phase space $h_{\epsilon,\epsilon',p} : \mathbb{R}^n \to \mathbb{R}^n$ mapping orbits of $\Sigma_{1,\epsilon}(p)$ at parameter p onto orbits of $\Sigma_{1,\epsilon'}(p')$ at parameter $p' = h_{\epsilon,\epsilon'}(p)$, preserving the direction of time.*

The following theorem states that the one-parameter bifurcation diagram of Σ_1 limits to the one-parameter bifurcation diagram of Σ_2 through a surjective but noninjective mapping, i.e. all transitions in the bifurcation diagram of Σ_1 are present in the bifurcation diagram of Σ_2, but some may take place simultaneously. In the theorem we denote by $(\cdot, \cdot)$ an open interval.

Theorem 2. *Consider systems Σ_1 and Σ_2 of Theorem 1, and let p be a parameter of f^+ and f^-. Take two continuous functions $p_L(\epsilon) : [0, \epsilon_{\max}] \to \mathbb{R}$ and $p_H(\epsilon) : [0, \epsilon_{\max}] \to \mathbb{R}$, with $p_L(\epsilon) < p_H(\epsilon)$ for all $\epsilon \in [0, \epsilon_{\max}]$. Let the homeomorphism $h_{\epsilon,\epsilon'}$ of Definition 4 be surjective from $(p_L(\epsilon), p_H(\epsilon))$ to $(p_L(\epsilon'), p_H(\epsilon'))$ for all pairs $\{\epsilon, \epsilon'\}$. Assume that*

(a1) for all $\epsilon, \epsilon' \in (0, \epsilon_{\max}]$, the families of systems $\Sigma_{1,\epsilon}(p)$, $p \in (p_L(\epsilon), p_H(\epsilon))$ and $\Sigma_{1,\epsilon'}(p)$, $p \in (p_L(\epsilon'), p_H(\epsilon'))$ are topologically equivalent;

(a2) the homeomorphism $h_{\epsilon,\epsilon'}$ between the parameter spaces of $\Sigma_{1,\epsilon}$ and $\Sigma_{1,\epsilon'}$ is continuous in $|\epsilon - \epsilon'|$ and equal to the identity at $\epsilon = \epsilon'$.

(a3) the homeomorphism $h_{\epsilon,\epsilon'}$ between the parameter spaces of $\Sigma_{1,\epsilon}$ and $\Sigma_{1,\epsilon'}$ is Lipschitz in p with Lipschitz constant independent of ϵ.

Then for any $\epsilon \in (0, \epsilon_{\max}]$

- *there exists a continuous but not necessarily invertible map $\mathcal{H}_\epsilon : [p_L(\epsilon), p_H(\epsilon)] \to [p_L(0), p_H(0)]$, $p' = \mathcal{H}_\epsilon(p)$, and*

- *there exists a map* $\mathcal{H}_{\epsilon,p} : \mathbb{R}^n \to \mathbb{R}^n$*, not necessarily invertible in* $\mathbf{x}$*, mapping orbits of* $\Sigma_{1,\epsilon}(p)$ *at parameter* p *onto orbits of* $\Sigma_2(p')$ *at parameter* $p' = \mathcal{H}_\epsilon(p)$*.*

Sketch of proof. Using Assumptions (a1) and (a2), for any $\Sigma_{1,\epsilon^*}(p)$ we can construct a path $p(\epsilon) : (0, \epsilon^*] \to \mathbb{R}$ such that all $\Sigma_{1,\epsilon}(p(\epsilon))$ are topologically equivalent systems. The map $\mathcal{H}_\epsilon(p)$ is the limit of $h_{\epsilon,\epsilon'}$ as $\epsilon' \to 0$, and is continuous being a limit of a sequence of Lipschitz maps (a3). Then, by Theorem 1, each orbit of $\Sigma_{1,\epsilon}(p(\epsilon))$ uniformly converges to an orbit of $\Sigma_2(p(0))$ as $\epsilon \to 0$. The induced map is the map $\mathcal{H}_{\epsilon,p}$. □

Acknowledgement

This research was partially done whilst the author was a visiting Researcher at the Centre de Recerca Matem‘atica in the Intensive Research Program on Advances in Nonsmooth Dynamics.

References

[1] A. F. Filippov. *Differential Equations with Discontinuous Righthand Sides*. Kluwer Academic Publishers, Dordrecht, 1988.

[2] Yu. A. Kuznetsov. *Elements of Applied Bifurcation Theory*. Springer-Verlag, Berlin, 3rd edition, 2004.

[3] J. Sotomayor and M. A. Teixeira. Regularization of discontinuous vector fields. In *Proceedings of the International Conference on Differential Equations, Lisboa*, pages 207–223, 1996.

Numerical treatment of reaction-diffusion problems with discontinuous forcing terms

Raffaele D'Ambrosio
Università degli Studi di Salerno
Via Giovanni Paolo II, 132, 84084 -Fisciano Italy
rdambrosio@unisa.it

Abramo Agosti
Politecnico di Milano
Via Bonardi, 9 - 20133 Milano, Italy
abramo.agosti@polimi.it

Luca Formaggia
Politecnico di Milano
Via Bonardi, 9 - 20133 Milano, Italy
luca.formaggia@polimi.it

Bianca Giovanardi
Politecnico di Milano
Via Bonardi, 9 - 20133 Milano, Italy
bianca.giovanardi@polimi.it

Anna Scotti
Politecnico di Milano
Via Bonardi, 9 - 20133 Milano, Italy
anna.scotti@polimi.it

The talk is focused on the numerical solution of reaction diffusion problems

$$\frac{\partial u}{\partial t} = \Delta u + f(u),$$

where the forcing term $f(u)$ is assumed to be discontinuous. Such a discontinuity is arisen by the presence of time-dependent thresholds which may or may not be also state-dependent. We introduce a numerical scheme obtained by a spatial discretization via linear finite elements, combined with a time discretization through suitable Runge-Kutta methods.

Due to the discontinuous nature of the problem, the introduced scheme is event driven. The selection of a suitable forcing term when the trajectories reach the discontinuity manifold is discussed. In particular, when the trajectory intersects the discontinuity manifold, in isolated points as well as in case of sliding motion, the selected vector field is the classical Filippov vector field generated as convex combination of the source terms defined outside the discontinuity. The scheme is also enriched by projection steps on the discontinuity, ensuring the convergence of the overall numerical scheme with the prescribed order of convergence, without loss of accuracy. Cases where the dynamics exhibits both

sliding and crossing modes are discussed. A selection of numerical experiments supporting the effectiveness of the approach is also shown.

References

[1] Dieci L. and Lopez L. Sliding motion in Filippov differential systems: Theoretical results and a computational approach. SIAM J. Numer. Anal., 47(3), 2023–2051 (2009).

[2] Filippov A.F. Differential Equations with Discontinuous Right-Hand Sides. Mathematics and Its Applications, Kluwer Academic, Dordrecht (1988).

Stable sliding solutions of discontinuous dynamical systems

Cinzia Elia
Università degli Studi di Bari
via Orabona, 4 70125 - Bari Italy
cinzia.elia@uniba.it

Luca Dieci
Georgia Institute of Technology
Atlanta, Georgia, USA
dieci@math.gatech.edu

Luciano Lopez
Università degli Studi di Bari
via Orabona, 4 70125 - Bari Italy
luciano.lopez@uniba.it

In this talk we examine the behavior of the trajectories of a piecewise smooth system in the neighborhood of a co-dimension 2 discontinuity manifold Σ. It is well known that if Σ is attractive (in the class of Filippov vector fields, and under commonly occurring conditions) one may anticipate sliding motion on Σ. However, this motion itself is not in general uniquely defined, and recent contributions in the literature have been trying to resolve this ambiguity either by justifying a particular selection of a Filippov vector field or by means of a suitable regularized problem. In this talk our concern is different: our ultimate goal is to detect properties that are satisfied by a sufficiently wide class of solutions of the discontinuous system regardless of the chosen sliding vector field. With this in mind, we will characterize stable sliding solutions of the discontinuous problem and relate them to the attractivity of Σ. With the aid of singular perturbation we will compare the behavior of stable solutions with the one of certain regularized solutions.

References

[1] L. Dieci, C. Elia, and L. Lopez, A Filippov sliding vector field on an attracting co-dimension 2 discontinuity surface, and a limited loss-of-attractivity analysis. *J. Differential Equations*, **254** (2013), 1800–1832.

[2] L. Dieci, C. Elia, and L. Lopez, Uniqueness of Filippov sliding vector field on the intersection of two surfaces in $\mathbb{R}^3$ and implications for stability of periodic orbits. *J. Nonlin. Science*, **25-6** (2015), 1453–1471.

[3] L. Dieci, and C. Elia, Discontinuous dynamical systems near a co-dimension 2 discontinuity manifold: can one say what should happen? *Discrete and Continuous Dynamical Systems-S*, Accepted.

A numerical procedure for geochemical compaction in the presence of discontinuous reactions

Bianca Giovanardi
MOX, Department of Mathematics, Politecnico di Milano
Via Bonardi, 9 20133 - Milano Italy
bianca.giovanardi@polimi.it

Abramo Agosti
MOX, Department of Mathematics, Politecnico di Milano
Via Bonardi, 9 20133 - Milano Italy
abramo.agosti@polimi.it

Luca Formaggia
MOX, Department of Mathematics, Politecnico di Milano
Via Bonardi, 9 20133 - Milano Italy
luca.formaggia@polimi.it

Anna Scotti
MOX, Department of Mathematics, Politecnico di Milano
Via Bonardi, 9 20133 - Milano Italy
anna.scotti@polimi.it

The process that transforms sediments into rocks involves complex physical mechanisms [4], namely mechanical compaction of the sediment solid matrix and chemical reactions. Mechanical compaction takes place over the million years, as the sediments are buried progressively deeper and the increased overload of the newly deposited material crushes and rearranges the grains, expelling part of the inter-pore fluid, thus reducing porosity and permeability. The chemical reactions, which cause the mineral to dissolve and precipitate [3], influence compaction by affecting the solid matrix porosity. Indeed, the dissolving mineral may leave some void spaces, whereas the precipitating mineral may fill them.
On the one hand, the variation of permeability resulting from the chemical reactions alters the pore pressure distribution linked to the flow of water through the rock and, as a consequence, the effective stress, thus counteracting or favoring mechanical compaction. On the other hand, the chemical reactions are influenced by the fluid flow itself, which transports the solute. The result is a nonlinear system of strongly coupled equations.
We present a numerical strategy to simulate the coupled problem of flow, compaction and reaction, focusing on the discontinuous nature of the differential equations that model the chemical reactions. In particular, we treat the discontinuous right hand side of the PDE for the solute by means of specially tailored event-driven numerical schemes *à la* [1]. These techniques, originally proposed and developed for the solution of ODEs, have the advantage of gaining accuracy and avoiding nonphysical solutions, such as negative concentrations and oscillations.
To this purpose, we introduce a splitting between the advection-diffusion part and the reaction term to take advantage of the event-driven methods proposed in [2], which allow

to localize the discontinuity in the reactions up to a prescribed tolerance. Our aim is to show by numerical experiments on several test cases that the present technique is not only suitable for the given problem but provides a more robust scheme with respect to standard solutions based on the regularization of the right hand side.

References

[1] L. Dieci, L. Lopez. 2012. *A survey of numerical methods for ivps of odes with discontinuous right-hand side*. Journal of Computational and Applied Mathematics. 236 (16), 3967–3991.

[2] L. Dieci, L. Lopez. 2013. *Numerical solution of discontinuous differential systems: Approaching the discontinuity surface from one side*. Applied Numerical Mathematics. 67, 98–110.

[3] A. C. Fowler, X. Yang. 2003. *Dissolution/precipitation mechanisms for diagenesis in sedimentary basins*. Journal of Geophysical Research: Solid Earth. 108.

[4] M. Wangen. 2010. *Physical principles of sedimentary basin analysis*. Cambridge University Press.

Time-transformations for the event location in discontinuous ODEs

Stefano Maset
Dipartimento di Matematica e Geoscienze - Università di Trieste
via Valerio, 12/1 34127 - Trieste Italy
maset@units.it

Luciano Lopez
Dipartimento di Matematica - Università di Bari
Via Edoardo Orabona, 4 70126 - Bari Italy
luciano.lopez@uniba.it

In this talk, we consider numerical methods for the location of events of ordinary differential equations

$$\begin{cases} x'(t) = f(x(t)), \ t \geq 0, \\ x(0) = x_0, \end{cases} \tag{1}$$

based on particular changes $t = \alpha(s)$ of the independent variable t, called time-transformations. Such a time-transformation reduces the integration of (1) up to the unknown point t_f where the event

$$h(x(t)) = 0$$

occurs, to the integration of a transformed equation

$$\begin{cases} \begin{bmatrix} y'(s) \\ \alpha'(s) \end{bmatrix} = \frac{\kappa'(s)}{h'(y(s))f(y(s))} \begin{bmatrix} f(y(s)) \\ 1 \end{bmatrix}, \ s \in [s_0, 0], \\ \begin{bmatrix} y(s_0) \\ \alpha(s_0) \end{bmatrix} = \begin{bmatrix} x_0 \\ 0 \end{bmatrix} \end{cases} \tag{2}$$

where κ is a given function and $s_0 = \kappa^{-1}(h(x_0))$. The point t_f and the value $x(t_f)$ are then recovered by

$$t_f = \alpha(0) \ \text{ and } \ x(t_f) = y(0).$$

Now, a standard numerical method is used for the integration of (1).
This approach was used in the context of delay differential equations in [1, 2], generalizes an approach presented in [3] and permits, amongst other things, to deal with situations where the solution lands on the surface $h(x) = 0$ in a tangential way.

References

[1] H. Brunner and S. Maset. Time transformations for delay differential equations. Discrete and Continuous Dynamical Systems, vol. 25 (3), pp. 751-775, 2009.

[2] H. Brunner and S. Maset. Time transformations for state dependent delay differential equations. Communication on Pure and applied Analysis, vol. 9 (1), pp. 23-45, 2010.

[3] L. Dieci and L. Lopez. One-Sided Direct Event Location Techniques in the Numerical Solution of Discontinuous Differential Systems. BIT Numerical Mathematics, vol. 55 (4), pp. 987-1003, 2015.

New Runge-Kutta methods for the one sided solution of discontinuous differential systems

Luis Rández
Universidad de Zaragoza
Pedro Cerbuna, 12 50009 - Zaragoza Spain
randez@unizar.es

Manuel Calvo
Universidad de Zaragoza
Pedro Cerbuna, 12 50009 - Zaragoza Spain
calvo@unizar.es

Juan I. Montijano
Universidad de Zaragoza
Pedro Cerbuna, 12 50009 - Zaragoza Spain
monti@unizar.es

Many real life processes are modeled by differential systems in which the vector field is non smooth. Such systems appear for example in electrical circuits, mechanical systems with friction, vehicle control or biology (see for example [1]). Some of these systems present in their dynamics sliding motion that is modeled by Filippov solutions. The discontinuity points (also called switching points) are characterized usually by a smooth function $g : \Sigma = \{y \in \mathbb{R}^n : g(y) = 0\}$ that defines a manifold and the vector field of the differential equation has locally different definitions at each side of the manifold. For example, the differential system for points such that $g(y) > 0$ can be defined as $y' = f_1(y)$ whereas for points with $g(y) < 0$ it is $y' = f_2(y)$. Then, the solution advances with time on one side of the manifold obeying a vector filed $f_1(y)$ until it reaches the switching manifold at a discontinuity point, and after that the solution continues on the other side of the manifold with $f_2(y)$ or else it stays onto the manifold in the case of a Filippov solution.
In order to integrate numerically these problems a precise location of the switching points is crucial. The computation of these switching points requires the solution of a nonlinear equation. However, recently L. Dieci and L. Lopez have proposed [3] a new technique that allows the computation of these switching points in an explicit way, by making a change of variables in the differential equations. The vector fields $f_1(y)$ or $f_2(y)$ can not be defined at the other side of the manifold and in this case, the design of special Runge-Kutta methods, called one-sided methods, for which it is guaranteed that in a step the internal stages remain all of them at the same side of the switching manifold, is required. L. Dieci and L. Lopez [2] have studied one sided Runge-Kutta methods and have given conditions to ensure that the internal stages lie on the same side of the switching manifold.
In this talk we propose the construction of Runge-Kutta methods for which it is guaranteed that all the internal stages are located at the same side of the switching manifold, for small enough step size, for any switching surface.

References

[1] di Bernardo, M., Budd, C. J., Champneys, A. R. and Kowalczyk, P. *Piecewise-smooth dynamical systems: Theory and applications.*. Applied Mathematical Sciences, Vol. 163. Springer-Verlag London, Ltd.

[2] Dieci, L. and Lopez, L. 2013 *Numerical solution of discontinuous differential systems: Approaching the discontinuity surface from one side*. Appl. Numer. Math. 67, 98–110.

[3] Dieci, L. and Lopez, L. 2015 *One-Sided Direct Event Location Techniques in the Numerical Solution of Discontinuous Differential Systems*. BIT 55, 4, 987–1003.

Applications of Operations Research

PROPOSERS

Federico Malucelli
Politecnico di Milano
DEIB, Piazza L. da Vinci 32, 20133 - Milano Italy
federico.malucelli@polimi.it

SPEAKERS

Maria Teresa Vespucci
Dipartimento di Informatica, Università di Bergamo
maria-teresa.vespucci@unibg.it

Andrea Taverna
DTI, Università di Milano
andrea.taverna@unimi.it

Roberto Zanotti
Università di Brescia
andrea.taverna@unimi.it

Stefano Gualandi
Dipartimento di Matematica, Università di Pavia
stefano.gualandi@gmail.com

Maurizio Bruglieri
INDACO, Politecnico di Milano
maurizio.bruglieri@polimi.it

Federico Malucelli
DEIB, Politecnico di Milano
federico.malucelli@polimi.it

The minisymposium will address some challenging applications of operations research methods in the field of energy, logistics and transportation.

References

[1] Bruglieri, M., A. Colorni, F. Lia "A multiobjective vehicle routing problem with time windows in last-mile logistics"

[2] Ceselli, A., G. Righini, D Siface , A. Taverna, "Ottimizzazione su larga scala dello Unit Commitment Problem per la simulazione a medio termine dei Sistemi Energetici"

[3] Gualandi, S. "A vehicle routing problem arising in the distribution of gasoline"

[4] Malucelli, F., E. Tresoldi, 'Disruption Management in local public transportation: the case of ATM"

[5] Mansini, R., M. Zanella, R. Zanotti "Scheduling and optimization: the case study of a wellness center"

[6] Vespucci, M.T., P. Piscella, D. Moneta, G. Viganò, "Optimal operation of power distribution networks with RES generation and storage devices"

Optimal operation of power distribution networks with RES generation and storage devices

Maria Teresa Vespucci
Università degli Studi di Bergamo
via Marconi 5 - 24044 Dalmine (BG), Italy
maria-teresa.vespucci@unibg.it

Paolo Pisciella
Università degli Studi di Bergamo
via dei Caniana 2 - 24127 Bergamo, Italy
paolo.pisciella@unibg.it

Diana Moneta
RSE - Ricerca sul Sistema Energetico S.p.A. - Milano, Italy
via Rubattino - 20134 Milano, Italy
Diana.Moneta@rse-web.it

Giacomo Viganò
RSE - Ricerca sul Sistema Energetico S.p.A. - Milano, Italy
via Rubattino - 20134 Milano, Italy
giacomo.vigano@rse-web.it

The operation of electricity Distribution Networks is going to change as a consequence of the large penetration of distributed generation, i.e. power plants (wind, photovoltaic, micro-CHP,…) directly connected to distribution networks. Distribution networks will host both dispatchable power plants (e.g. thermal), for which the production schedule is determined one day ahead by the plant's owner on the basis of load and price forecast, and non-dispatchable power plants (wind, photovoltaic), for which in advance only production forecasts are available, on the basis of weather forecast (wind speed, solar irradiance). As power generated by non-dispatchable plants is partially unpredictable, imbalance between load and generation is very likely to occur.
A new operator, the Distribution System Operator (DSO), will be in charge of operating the distribution network, in order to compensate generation-load imbalances, while guaranteeing technical feasibility, i.e. constraints on currents in lines (security) and voltages at nodes (power quality). Internal (i.e. owned by DSO) regulation resources will be electricity storage devices and on-load tap changers. DSO's external regulation resources (i.e. owned by third parties) will be exchanges of active and reactive power with the high voltage transmission network and dispatch of active and reactive power of generation plants. Costs associated to the use of internal regulation resources reflect device deterioration; costs associated to the use of external regulation resources have to be defined by the Regulator, so as to allow a technically efficient operation of the network. In this paper we introduce a two-step procedure for determining DSO's control actions for optimally operating a distribution network. The procedure can also be used as a simulation tool by the DSO to find efficient configurations of the network (e.g. determine effective

positions of storage units) and to analyze the impact of alternative sets of regulation resources. Moreover, the procedure can be used as a simulation tool by the Regulator to analyze the impact of different costs associated to external regulation resources.

Large-Scale Optimization of the Unit Commitment Problem for Medium-Term Energy Systems Simulations

Andrea Taverna
Università degli Studi di Milano - Dipartimento di Matematica
Via Cesare Saldini, 50, 20133 Milano
andrea.taverna@unimi.it

Alberto Ceselli
Università degli Studi di Milano - Dipartimento di Informatica
Via Bramante, 65, 26013 Crema, Italy
alberto.ceselli@unimi.it

Giovanni Righini
Università degli Studi di Milano - Dipartimento di Informatica
Via Bramante, 65, 26013 Crema, Italy
giovanni.righini@unimi.it

Dario Siface
Ricerca sul Sistema Energetico - RSE SpA
Via Rubattino, 54 20134 Milan, Italy
dario.siface@rse-web.it

The Unit Commitment Problem (UCP) computes an optimal schedule for thermal power plants to satisfy several system-wide constraints.
The model is used here to simulate the ideal behaviour of large-scale Energy Systems [1], spanning one or more countries, over one year with hourly resolution. Simulations are used by domain experts to evaluate different scenario hypothesis and support long-term decisions.
The model is formulated as a Large-Scale Mixed Integer Linear Problem (MILP) and includes different types of power plants and a transmission network.
The exact solution of the model is know to be impractical. We propose two approaches: a fast matheuristic, which employs continuous relaxations and spatial decomposition, and an exact approach based on column generation techniques. In the latter approach numerical instabilities, primarily due to degeneracy and objective function flatness, are often encountered while solving the master problem. To stabilize the algorithm we devise an ad-hoc dual LP optimization scheme based on Lagrangean Decomposition.
Experimental results on real-world data show that accurate results can be obtained by our framework in affordable time.

References

[1] Florian U. Leuthold, Hannes Weigt, and Christian Hirschhausen. A large-scale spatial optimization model of the european electricity market. *Networks and Spatial*

Economics, 12(1):75–107, 2010.

Optimizing the daily schedule of a wellness center

Roberto Zanotti
Università degli Studi di Brescia
via Branze, 38 25121 - Brescia Italy
r.zanotti003@unibs.it

Renata Mansini
Università degli Studi di Brescia
via Branze, 38 25121 - Brescia Italy
renata.mansini@unibs.it

Marina Zanella
Università degli Studi di Brescia
via Branze, 38 25121 - Brescia Italy
marina.zanella@unibs.it

Villa Paradiso is a wellness center on Garda Lake in Italy. A major task the hotel staff has to accomplish every day is scheduling the wellness activities for the next day. This task is time-consuming since it takes from three to five person-hours a day. In order to reduce this time (and possibly improve the quality of the resulting timetable), the hotel management would offer its staff an automatic support to solve the scheduling problem. The problem involves some entities: *Villa Paradiso* hosts from 20 to 50 guests, say *customers*, who can choose among 50 available wellness activities, say *services*, provided by approximately 20 *employees*. Every day each customer applies for his/her own set of services for the next day. Each service is provided by an employee. Services are partitioned into *categories*. Each employee is qualified to provide only the services falling into a specific category. An employee for each category is usually entrusted with providing a customer with all the services s/he is qualified for. A service is usually provided separately by an employee to a (single) customer. However, some services can simultaneously be provided to several customers. A default time length is assigned to each service. However, every time a customer applies for a service, s/he is allowed to ask for a non standard length. A hard time window is associated with each service. Any service, in order to be provided, may need one or more non-human resources, the amount of which is limited. Furthermore, each customer may express some preferences about his/her daily schedule, related, for example, to the ordering of the services or their specific allotted time intervals. There are about 10 different types of preferences that a customer can express. Additionally, the management of *Villa Paradiso* has issued a collection of guidelines that aims at improving the quality of the customers' daily schedules. The construction of the daily schedule has to push several aims. Maximizing the number of allocated services and satisfied customer preferences is the main goal of the scheduling task. The same applies to the guidelines specified by the wellness center, although their priority is lower than the ones of the customer preferences. *Villa Paradiso* is also interested in minimizing the idle time of both employees and customers.
Differently from what is usually done in the literature, we tackle this problem by adopting a mathematical programming approach. We have built a model to represent the core

problem and a set of constraints has been added for each type of preference (customers wishes or guidelines). In order to comply with the multi-objective nature of the problem, a 5 phases solving approach has been proposed. The model is used throughout every phase of the algorithm. A different objective function is considered at each stage, forcing the best solution values found in the previous stages as constraints for the following ones. This approach suits our needs the best, since the objectives are hierarchically ordered. In the first three phases, we aim at identifying the maximum number of jointly satisfiable soft constraints (preferences and guidelines). In fact, the problem instance obtained by including all the constraints may not be feasible and the algorithm has to decide which constraints to drop or to relax. The goal of the last two phases is to improve the overall quality of the solution, by reducing the customers' and employees' idle time. We show that, in all tested instances, the solution provided by our approach outperforms the one found by the center staff, in terms of satisfied customer preferences, satisfied guidelines and amount of idle time.

Vehicle routing for the heating oil industry

Stefano Gualandi
AntOptima, SA
via Aprica, 26, Lugano, Svizzera
stefano.gualandi@antoptima.com

L.M. Gambardella
AntOptima, SA
via Aprica, 26, Lugano, Svizzera
luca.gambardella@antoptima.com

In this work, we present a few challenges we faced in applying academic results on vehicle routing problems to practice. We focus on routing problems in the fuel distribution industry, where new orders for different type of heating oil products are continually arriving and the delivery of orders are planned using a fleet of heterogeneous vehicles placed at different depots. We discuss how optimization algorithms are embedded in a software application in order to: (1) assist the dispatcher to plan the fleet routes while respecting all operational constraints, and (2) support the commercial agents to place new orders in order to facilitate the route planning phase.
Our approach to solve the routing problem has three different stages.
In the first stage, we apply a construction heuristic inspired by the insertion heuristic introduced by Solomon [1]. Every day, a given number of different vehicles can be used; once the vehicles available for a given day are completely filled, the algorithms "opens" a new day and continues to construct tours: in practice, the number of vehicles is unlimited. However, differently from the Solomon's algorithm, we have for each order a double time window: the first time window specifies the range of days in which the order can be delivered, and the second time window limits the hours of the day in which the order must be delivered. The "day" time window can be violated, that is, the order can be delivered after its due date, but this comes with a penalty cost which must be minimized. In the insertion heuristic, we must consider that every driver, and hence every tour, has to include a lunch break of exactly one hour, which can start only between 12:00 and 12:15, and can occur only at specific locations. Each vehicle performs several trips during a working day, and, while it starts and finish the day at the same parking depot, during the day can be refilled at different depots. In the second stage of the routing algorithm, the application runs a simulated annealing heuristic starting from the solution obtained by the construction heuristic. The core of the simulated annealing is composed by different local search operators, which are extended versions of the traditional operators reviewed in [2]. In this second stage, the algorithm tries first to minimize the number of orders that are delivered after theirs due date, and, as secondary objective, it tries to minimize the total tours length.
In the last third stage, we apply a post processing algorithm that for each single tour runs an exact branch-and-bound algorithm to solve a Travelling Salesman Problem with Time Window [3] defined only over the orders assigned to that vehicle.
Once the route planner has completed the three stages and it has found a solution, using our desktop application, the user can modify the solution by dragging-and-dropping

orders from one tour to the other, by adding to tours new orders that are arrived in the meantime, or by building tours that violate one or more constraints. The user can block any tour he has modified, and he can run our route planner again and again, eventually running only the second and third stage of our route planner.
The solution we have developed is used every day by our customer, and it has been used to route up to 1500 orders in less than a minute.

References

[1] Solomon, Marius M. 1987 *Algorithms for the vehicle routing and scheduling problems with time window constraints*. Operations research, vol. 35(2), 254–265.

[2] Savelsbergh, Martin WP. *Local search in routing problems with time windows*. Annals of Operations research, vol. 4(1), 285–305.

[3] Dumas, Yvan and Desrosiers, Jacques and Gelinas, Eric and Solomon, Marius M. 1995 *An optimal algorithm for the traveling salesman problem with time windows*. Operations research, vol. 33(2), 367–371.

A Multiobjective Vehicle Routing Problem With Time Windows In Last-Mile Logistics

Maurizio Bruglieri
Politecnico di Milano
via Durando, 38/a 20158 - Milano Italy
maurizio.bruglieri@polimi.it

Alberto Colorni
Politecnico di Milano
Via Durando, 38/a 20158 - Milano Italy
alberto.colorni@polimi.it

Federico Lia
Consorzio Poliedra - Politecnico di Milano
via G. Colombo, 40 20133 - Milano Italy
federico.lia@polimi.it

The growth in the volume of freight traffic, as well as environmental and traffic congestion reasons, has led in recent years to a switch of distribution strategy from the direct shipping to systems where freight is delivered to the customers through intermediate depots, so called Urban Satellite Platforms (USPs). In the USPs, the parcels, that previously traveled on trucks, are disaggregated and reassigned to lighter and environmentally sustainable vehicles (e.g. electric vans and cargo-bike) for urban center deliveries.
In this context we addressed inside the project OPTILOG (OPTImal and sustainable LOGistics in urban areas), financed by Lombardia Region (Italy), a particular optimization problem arising in last-mile logistics. A set of long-haul carriers (LHC) and a set of last-mile carriers (LMC) are given. At an early accreditation stage, each LHC company must declare the set of LMC companies to which wants to consign its freight. In addition, some LHC companies may allow their products to travel in light vehicles along with those of the other LHCs, while others may require an exclusive transport service (mixing conditions).
Each LHCs' parcel is characterized by a destination address, a volume, a weight and a delivery time window (TW). Some deliveries can be optional in order to model parcels that must be delivered within a long period (e.g. a week): in this way, we avoid to directly handle a multi-period delivery problem, by making the shipment optional until its final delivery day is reached.
In each USP a fleet of heterogeneous vehicles belonging to different LMC companies, are present. Each vehicle is characterized by typology and capacity. Moreover each LMC has a favorite delivery zone, on the basis of the territory knowledge made with previous deliveries.
The problem that we want to solve is to decide how to assign the parcels to the USPs, and within each USP how to route and schedule each LMC taking into account the following constraints:

1. each LMC route must start and end in the belonging USP;
2. each LMC can ship only the parcels assigned to his USP;
3. vehicle capacity must not be exceeded;
4. delivery TWs must be respected;
5. route durations must not to exceed the duty time;
6. requirements of LHCs must be respected (i.e. LMC companies choice and mixing conditions).

Multiple objectives need to be optimized at the same time: minimize the LMCs employed, maximize the total number of optional shipments satisfied, minimize the total length of the vehicle routes, balance them as much as possible and maximize the preferences of LMCs. We obtain this, through the optimization of a single objective given by the weighted sum of the utility functions associated with each criterion.
Although our problem owns some similarities with the two-echelon vehicle routing problem (2E-VRP) [1], [2], it differs from it since we are not interested to determine the routes of the LHCs but only to assign their parcels to the USPs. Moreover, features as delivery TW, optional deliveries, heterogeneous fleet, LHCs' requirements and LMCs' preferences are not usually considered in the 2E-VRP. The latter feature can instead be modeled as incompatible loading constraint [3].
For this problem we present a Mixed Integer Linear Programming (MILP) formulation. Moreover, we also develop a heuristic approach in order to face real world alike instances derived from the Milan road network.

References

[1] Hemmelmayr, V. C., Cordeau, J. F., Crainic, T. G. *An adaptive large neighbourhood search heuristic for Two-Echelon Vehicle Routing Problems arising in city logistics.* Computers & Operations Research 39 (2012), 3215–3228.

[2] Perboli, G., Tadei, R., Vigo, D., *The two-echelon capacitated vehicle routing problem: models and math-based heuristics*, Transportation Science 45 (2011), 364–380.

[3] Wang, Z., Li, Y., Hu, X. *A heuristic approach and a tabu search for the heterogeneous multi-type fleet vehicle routing problem with time windows and an incompatible loading constraint*, Computers & Industrial Engineering 89 (2015), 162–176.

Disruption Management in local public transportation: the case of ATM

Federico Malucelli
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
federico.malucelli@polimi.it

Emanuele Tresoldi
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
emanuele.tresoldi@polimi.it

The quality of a local public transport depends on the perceived efficiency and reliability of the service. However, events or delays innate in the system, especially in a urban setting, may generate disruptions that negatively influence this perception and complicate the daily management. Additionally, disruptions usually increase the operating cost, for instance, involving extra allowances for bus drivers, or penalties to be payed to the municipality that commended the service.

The daily operations of transit companies are often monitored by an operation central office taking advantage of Automated Vehicle Monitoring (AVM) systems and mobile telecommunication devices. By means of AVM a huge amount of data is available but, in most of the cases, these data are used in a very limited extent. In the case of ATM of Milan, each operator visually controls the operations of one or more lines on a screen reporting in real time the vehicle positions on a map. The operators can detect from the screen delays or anomalies that may generate disruptions or they collect information from drivers about troubles on the line such as vehicle breakdowns, accidents or medical and safety emergencies. In the presence of a disruption, the operator assists remotely the drivers directly involved in the disruption, decides the actions to be taken coordinating, in case, also the behavior of the other drivers on the same line or other lines sharing a portion of the network with the disrupted one. In addition, the operator must inform passengers, both onboard and waiting at the stops, of the new solution adopted to tackle the disruption. The basic actions that an operator in the central office can evaluate are, for instance, to perform vehicle short-turns, to delay a vehicle, or to cancel one or more trips. The operator may also decide to use spare resources (drivers or vehicles). However, this is not an option for the ordinary disruption management since, usually, these resources are extremely scarce and are left for tackling exceptional cases only. Even though operators are very expert in recovering disruptions or preventing them, they usually have not the intuition on the effect of their interventions on the resource management, both vehicle and crew scheduling. This is because they are not enabled to have a full understanding of the effect of their actions on the vehicle and crew scheduling, and also because the task of adjusting manually the planned scheduling goes beyond their duty. Thus the effect of recovering a disruption in the morning may have an even worse disruptive effect later on when drivers duties come to an end.

These issues call for a thorough analysis of the problem and the study of optimization methods to be included into a decision support system to assist operators in taking decisions.

Disruption management in transportation is not a new subject. Methods to cope with disruptions have been introduced initially in the airline industry (see for example [4]) and then extended to railways ([3]). The complexity of the constraints emerging in railways, mainly due to the shared infrastructure, often suggested hybrid approaches conjugating optimization techniques with simulation ([2]). Only recently this problem has been tackled in local public transport. In this context, peculiar features motivate an ad hoc study of disruption management methods that can take advantage of transit additional flexibility such as trip cancellations, short-turns that add significant degrees of freedom and open for different types of approaches (see for example [1]).

In this work we present a tool that, exploiting the real time data, can assist the operators to face different types of small delays and disturbances with the ultimate objective of increasing the quality of service, or at least to limit the perception of inconvenience on passengers, using the available resources, and proposes a real time adjustment of vehicle and crew scheduling. We investigate the way ATM assesses the quality of the service and we propose improved methods for the evaluation of the regularity of the service. Then, we introduce the *Disruption-delay management framework* based on a discrete event simulator and on a tabu-search algorithm for the real-time re-scheduling of the vehicles. After that, we present the column generation method used to tackle the consequent crew scheduling re-optimization. Finally, we report the results obtained by our procedure in real-world scenarios arising in the urban management of surface lines of ATM.

References

[1] Bartholdi-III, J. J., and D. D. Eisenstein, 2012 *A self-coordinating bus route to resist bus bunching* Transportation Research Part B 46, 481–491.

[2] Berger,A., R. Hoffmann, U. Lorenz and S. Stiller, 2011 *Online railway delay management: Hardness, simulation and computation*, Simulation 87 (7) 616–629.

[3] Cacchiani, V., D. Huisman, M. Kidd, L. Kroon, P. Toth, L. Veelenturf and J. Wagenaar, 2014 *An overview of recovery models and algorithms for real-time railway rescheduling*, Transportation Research Part B 63, 15–37.

[4] Clausen, Jens, A. Larsen, J. Larsen and N.J. Rezanova, 2010 *Disruption management in the airline industryÑconcepts, models and methods* Computers & Operations Research, 37 (5) 809–821.

Application of Mathematical Methods in Petroleum Exploration

PROPOSERS

Edie Miglio
Politecnico di Milano
Pzza Leonardo da Vinci, 32 20133 - Milano, Italy
edie.miglio@polimi.it

Paolo Ruffo
Eni SpA Upstream and Technical Services, RIGE Dept.
Via Emilia, 1, 20097 San Donato Milanese (MI), Italy
paolo.ruffo@eni.com

SPEAKERS

Vittorio De Tomasi
Eni SpA Upstream and Technical Services, RIGE Dept.
vittorio.detomasi@eni.it

Cristiano Malossi
IBM Research, Zurich
acm@zurich.ibm.com

Mattia Penati
Dept. of Mathematics, Politecnico di Milano
mattia.penati@polimi.it

Didier Renard
Centre de Gèosciences, Fontainebleau
didier.renard@mines-paristech.fr

Kosuke Ueda
Institute of Geophysics, Department of Earth Sciences
kosuke.ueda@erdw.ethz.ch

The search for hydrocarbons in petroleum exploration is a complex activity that makes use of a range of mathematical tools in order to improve the probability of finding new reserves. These techniques ranges from the building of a numerical model of present day geology of the earth, in the area of interest, to that of modelling the most critical geological processes that have originated the present day geomodel.
In this minisymposium we aim at collecting contribution of different researches working on different mathematical and numerical methods used in petroleum engineering.
In particular the following problems will be considered:

- seismic processing techniques;
- basin evolution;

- plate tectonics;
- post glacial rebound;
- thermal effects;
- advanced spatial estimation/simulation techniques.

From the mathematical point of view the methods used in the above mentioned applications range from the inversion methods, mesh adaptation and geometry processing, numerical methods for visco-elasto-plastic materials, high performance computing for large scale simulations, phase transition problems and geostatistical methods.

On the estimation of the apparent oscillation frequency of a time series.

Vittorio De Tomasi
ENI, Upstream and Technical Services
via Emilia 1 – 20097 San Donato Milanese
vittorio.detomasi@eni.com

The estimation of the apparent or "instantaneous" oscillation frequency in a time series is an interesting problem that has many applications in science and engineering. Noise and non-stationarity issues make however the problem difficult to solve. A method often used in many applications is based upon modeling the time series as a complex signal (see [9]), i.e. by setting

$$y(t) = x(t) + ih(t) = A(t)e^{-i\phi((t)t}|_{t=0,\ldots,T} \tag{1}$$

$$\phi(t) = \text{atan}\left[\frac{\mathcal{I}}{\mathcal{R}}\right] \tag{2}$$

$$f(t) = \frac{1}{2\pi}\frac{\partial\phi(t)}{\partial t} \tag{3}$$

where $A(t)$ represents the local signal amplitude, $\phi(t)$ its phase, $h(t) = H[x(t)]$ is the Hilbert transform of $x(t)$ and $f(t)$ is the local (or "instantaneous") signal frequency. While the method seems obvious, its practical implementation is affected by several problems. Hilbert transform is usually computed by Fourier-transforming the sequence, nulling out spectrum for $f < 0$, and back transforming the data. This implicitly assumes that the signal is periodic, and an often overlooked point is the fact that the discrete Hilbert transform is approximate, and the error depends from some features of the signal itself (see [7]). Further problems arise from the calculation of the $\mathcal{I}/\mathcal{R}$ ratio and from numerical differentiation: these operations have the unwanted consequence of amplifying the noise intrinsic to the time series, so that the whole method becomes near useless for signals with a poor signal/noise ratio. Fomel suggested a method based upon Tikhonov regularization for stabilizing the estimation of frequency. Combining equations (1)-(3) one gets

$$f(t) = \frac{1}{2\pi}\frac{\partial\phi(t)}{\partial t} = \frac{1}{2\pi}\frac{x\frac{\partial h}{\partial t} - h\frac{\partial x}{\partial t}}{x^2 + xh^2} = \frac{F(t)}{G(t)} \tag{4}$$

This can be discretized as $W = G^{-1}F$, where the signal is discretized at time instants $n = \{0, \Delta t, 2\Delta t, ...(N-1)\Delta t\}$ with Δt being the sampling interval, G is a NxN diagonal matrix whose nonzero elements are equal to $A^2(n)$, and F is the $Nx1$ vector containing the samples of $f(t)$ to be determined. Tikhonov regularization requires the minimization of $\begin{bmatrix} GW - F \\ \varepsilon RW \end{bmatrix}$, whose solution is given by

$$W = \left(G^T G + \varepsilon^2 R^T R\right)^{-1} F \tag{5}$$

where R being the regularization operator. Fomel observed that in the general case of data smoothing $G = I$ and R is an appropriate smoothing operator. Defining $S = \left(I + \varepsilon^2 R^T R\right)$ the solution to (5) can be rewritten as:

$$W = \left[\varepsilon^2 I + S(G - \varepsilon^2 I)\right]^{-1} SF. \tag{6}$$

Fomel used a triangular smoothing operator (see [1]) for the conditioner S, i.e

$$S_{ij} = \begin{cases} |\frac{M-|j-i|}{M}| & M < \frac{N}{2}, |i-j| \leq M \\ 0 & \text{elesewhere} \end{cases} \tag{7}$$

$$\sum_{j=1}^{N} S_{ij} = 1$$

so matrix S is a banded matrix of bandwidth M (in this context the bandwidth is the number of nonzero elements in a row of S counting from the diagonal). However as shown by Fomel the use of a triangular smoothing operator for conditioning the frequency estimation results in a loss of time resolution, making the whole method unsuitable for most practical purposes. In a further paper ([6]) the method was used for conditioning the frequency estimation obtained with a time-frequency analysis: the results were quite satisfactory in terms of time and frequency resolution, but with a high computational cost. The method described in equations (1)-(6) is however appealing due to its simplicity: it was then analyzed to see if it could be modified by enhancing its time resolution, without sacrificing its noise immunity. By inspecting equation (6) it can be seen that operator S acts as a convolutional filter (see [8]) applied separately to the numerator and denominator of eq. (5). In practice, the purpose of S is to filter out the unwanted noise: the best estimate for the frequency is then obtained in the least square sense from the filtered $F(t)/G(t)$ ratio. There are two factors affecting time resolution of the algorithm. The first factor controlling resolution is the bandwidth M of matrix S: its rows act on the signal by mixing and averaging $F(t)$ and $G(t)$ before the least square estimation, so the smaller the value of M the higher the resolution. The second factor controlling the resolution is the frequency bandwidth of the operator used to construct the rows of matrix S (in this context "bandwidth" refers to the frequency spanned by the Fourier spectrum of $x(t)$). The triangular window operator (see (7)) adopted by Fomel is not the best filter to choose: it has strong secondary lobes, and its spectrum decays as $1/x$, so for best results a large M is needed for an efficient noise rejection. The solution is clearly to replace equation (7) with a better filtering operator with reduced side lobes, i.e. a FIR low pass filter whose cutoff frequency is appropriately tailored to the signal bandwidth. Given filter specifications (namely frequency cutoff and decay, and the filter order M) the impulse response $h(n)(n = -M/2, \ldots, M/2)$ of a FIR filter is calculated, and then $h(n)$ is used in place of eq. (7) for filling the rows of matrix S. It was found that the cutoff frequency of the filter is not very critical, and usually it is set close to the guessed oscillation frequency of the time series.

It is interesting to observe that while operator S in eq. (6) is represented as a linear operator, also a nonlinear operator could be used for filtering out the noise from the time series $F(t)$ and $G(t)$, like for example the median filter (see [3]) or a shrinkage operator (see [2]).

Figures 1-5 demonstrate the concepts described above: in particular Figure 1 compares the spectral response of eq. (7) against that of a FIR filter with the same M. The advantage

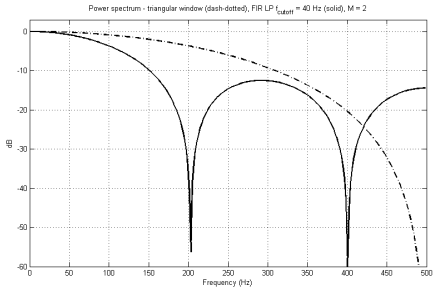


Figure 1: Comparison between traingular and FIR LP filter responses

of using a tailored FIR filter is evident. It can also be observed the fact that replacing eq. (7) with a low pass filter, besides increasing time resolution, results also in a better noise rejection. By increasing M, the performances of the triangular filter smoother and of the FIR filter, tend to converge to a common value, so the method proposed here is advantageous for small values of M.
We finally point out that equations (1)-(3) are not the only way to estimate the apparent frequency. These equations actually describe an unknown oscillating process as an harmonic oscillator (see [11]). From the theory of harmonic oscillations (see [5]) it can be shown that the frequency of oscillation is given by:

$$f = \frac{1}{2\pi}\sqrt{-\frac{\ddot{x(t)}}{x(t)}}. \tag{8}$$

So by setting $F(t) = \dfrac{\partial^2 x}{\partial t^2}$, $\quad G(t) = x(t)$, equation (6) can be used for estimating the apparent frequency from equation (8). The interesting point is that eq. (8) represents a "hilbertless" estimator of frequency, so the equation could be used for estimating the frequency of highly nonstationary signals. An example of the results obtained combining eq. (6) and (8) is shown in figures 2-5 together with the results obtained with the Hilbert-based frequency estimator. Some improvements are still needed, in order to take full advantage of Tikhonov regularization method applied to equation (8), but the preliminary results obtained appear to be encouraging.

Conclusions An estimation of apparent oscillating frequency from a time series is difficult to obtain when noise or non-stationarity are present. Tikhonov regularization can help to improve the estimation, if a suitable data regularization operator is found. Linear low pass filters tailored to the signal bandwidth or nonlinear denoising operators can be used as regularization operators, improving the estimation of the frequency without significantly degrading the time resolution. The regularization method can be applied to either Hilbert- or Hilbertless- frequency estimators.

Acknowledgments The author thanks ENI management for the permission of publishing this paper. A special thank goes also to Luca Mapelli and Gabriele Gambacorta, who proposed to the author the geophysical challenges that led to the development of this algorithm.

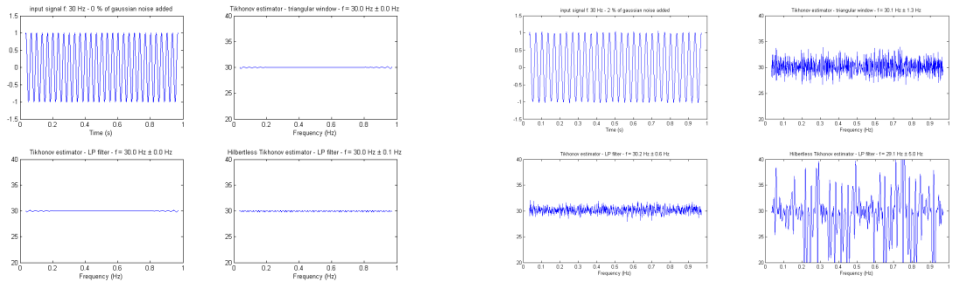


Figure 2: Estimation properties of the three algorithms with no noise (left) and 2% noise (right)

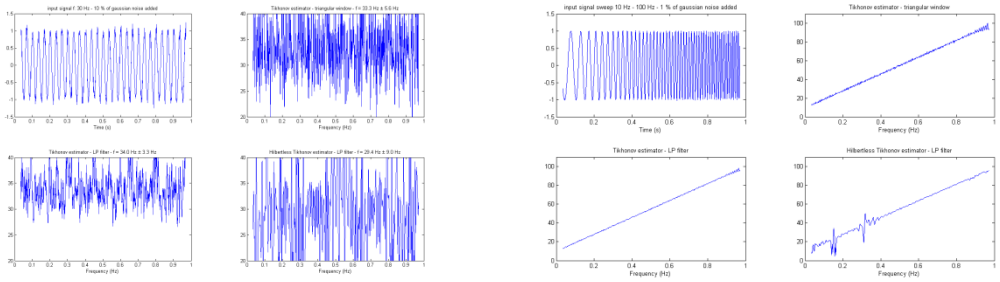


Figure 3: Estimation properties of the three algorithms with 10% noise (left) and 1% noise (right)

References

[1] Claerbout J. F. 1992 Earth Sounding Analysis: processing versus Inversion. Blackwell

[2] Donoho D. L., Denoising by soft thresholding, IEEE trans. on Information Theory 41 613-627

[3] Duncan G., Beresford G Median filter behavior with seismic data Geophysical Prospecting 43, 329-345

[4] Fomel, S. 2007 Local seismic attributes. Geophysics 72, A29-A33

[5] Landau L. D., Lifshitz E. M. 1969 Mechanics. Pergamon

[6] Liu G., Fomel S., Chen X. 2011 Time-frequency analysis of seismic data using local attributes Geophysics 76 P23-P24

[7] Nuttall A. H. 1966 On the quadrature approximation to the Hilbert transform of modulated signals, Proc. IEEE 54, 1458-1459

[8] Oppenheim A. V., Schafer R. W, 1975 Digital signal processing, Prentice Hall

[9] Taner, M. T., Koehler F., Sheriff R. E. Complex seismic trace analysis. Geophysics 44 1041-1063

[10] Tikhonov A.N. et al. 1990 Numerical Methods for the Solution of Ill-Posed Problems. Springer

[11] Ulrych, T.J. Sacchi M., Graul M., Taner M. T. 2007 Istantaneous attributes: the what and the how, Expl. Geophysics 38, 213-219

Extreme-Scale Earth's Mantle Flow Simulation on IBM BlueGene/Q

Cristiano Malossi
Foundations of Cognitive Solutions
IBM Research – Zurich, Switzerland
acm@zurich.ibm.com

Costas Bekas
bek@zurich.ibm.com

Yves Ineichen
yin@zurich.ibm.com

Peter Staar
taa@zurich.ibm.com

Alessandro Curioni
cur@zurich.ibm.com

Earth is a dynamic system in which mantle convection drives plate tectonics and continental drift and, in turn, controls much activity ranging from the occurrence of earthquakes and volcanoes to mountain building and long-term sea level change. Despite its central role in solid earth dynamics, we have enormous first-order gaps in our knowledge of mantle convection, with questions that are as basic as what are the principal driving and resisting forces on plate tectonics to what is the energy balance of the planet as a whole. Addressing these questions requires global models of earth's mantle convection and associated plate tectonics, with realistic parameters and high resolutions down to faulted plate boundaries. Historically, modeling at this scale has been out of the question due to the enormous computational complexity associated with numerical solution of the underlying mantle flow equations. However, with the advent of multi-petaflops supercomputers as well as significant advances in seismic tomography and space geodesy placing key observational constraints on mantle convection, we now have the opportunity to address these fundamental questions. Successful solution of realistic mantle flow problems must overcome a number of computational challenges due to the severe nonlinearity, heterogeneity, and anisotropy of earth's rheology. Nonlinear behavior at narrow plate boundary regions influences the motion of whole plates at continental scales, resulting in a wide range of spatial scales, thus adaptive methods are essential. Six orders of magnitude viscosity contrast is characteristic of the shear zones at plate boundaries, yielding sharp viscosity gradients and leading to severe ill-conditioning. Furthermore, the viscosity's dependence on a power of the second invariant of the strain rate tensor and plastic yielding phenomena lead to severely nonlinear behavior. Overcoming major obstacles in modeling and simulating such an extremely complex physical problem has been one of the main driving research activities of Prof. Omar Ghattas team over the last 10 years [1, 2, 3, 5]. In this work, we present the result of a two-years collaboration between his team and IBM

Research – Zurich, where the original methodology has tuned and re-engineered in a code able to make optimal use of the massively parallel characteristics of the IBM BlueGene/Q Sequoia system[3]. The results of this work demonstrate that—contrary to conventional wisdom—algorithmically optimal implicit solvers can be designed that scale out to 1.5 million cores for severely nonlinear, ill-conditioned, heterogeneous, and anisotropic PDEs. This work has been originally presented at SC'15 and awarded with the ACM Gordon Bell prize [4].

References

[1] Laura Alisic, Michael Gurnis, Georg Stadler, Carsten Burstedde, and Omar Ghattas. Multi-scale dynamics and rheology of mantle flow with plates. *Journal of Geophysical Research*, 117:B10402, 2012.

[2] Laura Alisic, Michael Gurnis, Georg Stadler, Carsten Burstedde, Lucas C. Wilcox, and Omar Ghattas. Slab stress and strain rate as constraints on global mantle flow. *Geophysical Research Letters*, 37:L22308, 2010.

[3] Carsten Burstedde, Omar Ghattas, Michael Gurnis, Tobin Isaac, Georg Stadler, Tim Warburton, and Lucas C. Wilcox. Extreme-scale AMR. In *Proceedings of SC10*. ACM/IEEE, 2010.

[4] Johann Rudi, A. Cristiano I. Malossi, Tobin Isaac, Georg Stadler, Michael Gurnis, Peter W. J. Staar, Yves Ineichen, Costas Bekas, Alessandro Curioni, and Omar Ghattas. An extreme-scale implicit solver for complex pdes: Highly heterogeneous flow in earth's mantle. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis*, SC '15, pages 5:1–5:12, New York, NY, USA, 2015. ACM.

[5] Georg Stadler, Michael Gurnis, Carsten Burstedde, Lucas C. Wilcox, Laura Alisic, and Omar Ghattas. The dynamics of plate tectonics and mantle flow: From local to global scales. *Science*, 329(5995):1033–1038, 2010.

[3] IBM and BlueGene are trademarks of International Business Machines Corporation, registered in many jurisdictions worldwide. Linux is a registered trademark of Linus Torvalds in the United States, other countries, or both. Other product or service names might be trademarks of IBM or other companies.

PoGlaR - A finite element code for high performance simulation of Post Glacial Rebound

Mattia Penati
MOX–Modellistica e Calcolo Scientifico, Dipartimento di Matematica, Politecnico di Milano
Piazza Leonardo da Vinci 32, 20133 Milano, Italy
mattia.penati@polimi.it

Edie Miglio
MOX–Modellistica e Calcolo Scientifico, Dipartimento di Matematica, Politecnico di Milano
Piazza Leonardo da Vinci 32, 20133 Milano, Italy
edie.miglio@polimi.it

Paolo Ruffo
Eni SpA Upstream and Technical Services, RIGE Dept.
Via Emilia, 1, 20097 San Donato Milanese (MI), Italy
paolo.ruffo@eni.com

From the mechanical point of view the interior of the Earth can be considered as composed of four main layers: the inner and outer core, the mantle and the lithosphere. The lithosphere can be assumed to be elastic and the solid mantle beneath behaves as a viscous fluid. The long term equilibrium pressure at a given depth in the Earth is due to the weight of the material above this depth. Deviations from this equilibrium state lead to material transport from regions of higher pressure towards lower pressure. If left undisturbed over time the mantle and the lithosphere reach an equilibrium, in which the depth of the base of the lithosphere will mainly depend on the thickness of the lithosphere. This phenomenon is due to the Archimedes principle stating that the mass of the volume of a fluid displaced by a floating object is equal to the mass of the object. In the Earth we refer to this as isostacy or isostatic equilibrium. The growth of ice sheets during a glacial period concentrates mass on the Earth's surface to glaciated areas; this fact increases the pressure in the layers below, resulting in a sinking of the lithosphere and in a transport of mantle material away from the region. At the end of the glacial period, when the ice sheets melt away, the pressure on the lithosphere is reduced and the material will flow back causing the surface to uplift. Compared to the water the mantle viscosity is 10^{22} to 10^{25} times higher, therefore the uplifting will be slow down and continue long time after the ice has gone. The entire process of subsidence during the glacial growth, followed by uplift during and after deglaciation, is referred as glacial isostatic adjustment and with the expression post-glacial adjustment we refer to the uplift phase. The influence of the glacial isostatic movements on the hydrocarbon bearing rocks has been investigated [3, 4, 5]. Even if among the petroleum geologists the effect has been almost neglected, Fjeldskaar shown that the this effect can be severe in flat and large structures [5]. By means of coupling the stratigraphic data from the Quaternary and latest Tertiary periods and realistic ice models the author has been able to show that as much as 30 % of the total hydrocarbon volume can be lost during the maximum glacial isostatic downwarping. Moreover the thermal consequences of taking glaciation

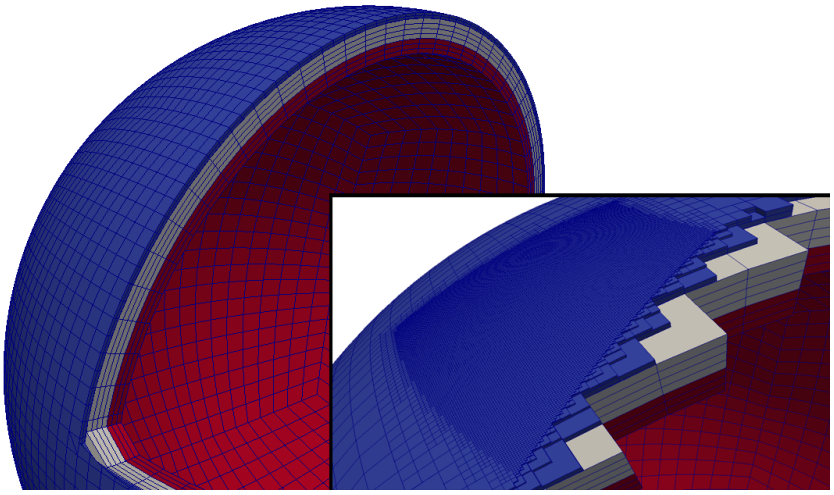


Figure 1: The mesh generated without refinement, the color represents the different layers of the model: litosphere, upper mantle and transition zone. In the smaller frame a detail of the refined mesh in a given region, the smallest cells have a resolution of about 20 km, the largest ones of 320 km.

into account can be significant as well; knowing which type of glacier is present at which time is crucial in order to have a good estimate of subsurface temperatures in glaciated areas [4]. PoGlaR is a C++ code for the simulation of the Post Glacial Rebound at global scale; this code is mainly based on the deal.II Finite Element Library [1]. It is a finite element parallel code for forward modelling of the viscoelastic response of a three dimensional elastically compressible Earth to an arbitrary surface load. The code is able to perform global simulation of the rebound process, with a more refined results on a selected geographical region. In order to perform such simulation in a reasonable time and with a good level of details the code has been designed to exploit all the levels of parallelism: both shared and distributed systems. The model implemented in PoGlaR consists of two parts: an Earth model and an ice reconstruction, where the latter is imposed as a boundary condition on the former. Different methods to set up the Earth model exist, while the ice reconstruction is usually based on observed data or taken from thermo-mechanical modeling. In the timescale of the post-glacial adjustment process the deformations of the Earth are viscoelastic. This means that when loaded the mantle initially responds like an elastic medium, then it flows like a viscous fluid over long timescales, but complications arise due to the presence of initial stress in the interior of the planet. The initial stress $t^{(0)}$ is assumed to be solution of a static equilibrium state and the Earth is assumed to be a fluid. Since the fluid at rest cannot maintain deviatoric stresses, the initial state must be an hydrostatic equilibrium state. Then the stress tensor is defined as $t^{(0)} = -p^{(0)}I$, where the pressure $p^{(0)}$ is the solution of the static problem:

$$\begin{cases} -\operatorname{grad} p^{(0)} + \rho^{(0)}\mathbf{g}^{(0)} = 0, \\ \mathbf{g}^{(0)} = \operatorname{grad} \phi^{(0)}, \\ -\Delta\phi^{(0)} = 4\pi G\rho^{(0)}, \end{cases}$$

where ρ denotes the density and ϕ the gravitational potential. The incremental stress $t^{(\delta)}$ is assumed to be solution of the Maxwell viscoelastic problem (or linear viscoelastic

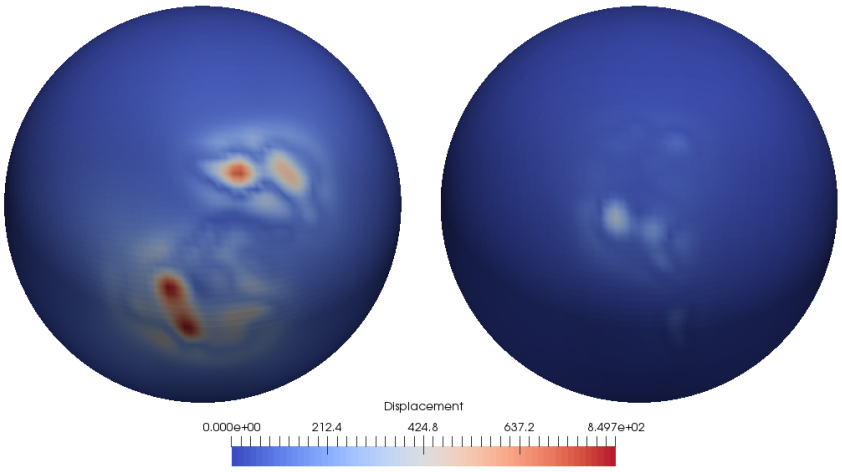


Figure 2: The displacemente magnitude in meter obtained using the mesh without refinement. The images represent the North and South poles respectively.

problem), it is defined by the following state equations

$$\begin{cases} t^{(\delta)} = 2\mu \operatorname{dev}(\operatorname{sym}\operatorname{grad}\mathbf{u}) + pI - q, \\ \dot{q} + \dfrac{1}{\tau}q = \dfrac{1}{\tau}2\mu \operatorname{dev}(\operatorname{sym}\operatorname{grad}\mathbf{u}), \\ \operatorname{div}\mathbf{u} = \dfrac{1}{K}p. \end{cases}$$

where $\mathbf{u}$ denotes the dispacement field. These equations are coupled with the equations of dynamics and for glacial isostatic adjustment problem are given by

$$\begin{cases} \operatorname{div} t^{(\delta)} + \operatorname{grad}(\operatorname{grad} p^0 \cdot \mathbf{u}) - \mathbf{g}^{(0)} \operatorname{div}(\rho^{(0)}\mathbf{u}) + \rho^{(0)}\mathbf{g}^{(\delta)} = 0, \\ \mathbf{g}^{(\delta)} = \operatorname{grad}\phi^{(\delta)}, \\ -\Delta\phi^{(\delta)} = -4\pi G \operatorname{div}(\rho^{(0)}\mathbf{u}). \end{cases}$$

The domain is assumed to be a layered WGS84 ellipsoid: the thickness and the material properties of each layer are taken from the PREM model [2]: a one dimensional averaged model representing the elastic properties inferred from the seismic data as a function of planetary radius. Richar Peltier is one of the most prolific author in the context of ice reconstruction; he proposed different models for reconstructing the climates [6, 7, 8] and the distribution of land ice that existed on the continents. The model included in the code is the ICE-5G model [8] developed by Peltier, a global model for the last glaciation based on the inversion of the relative sea level history and the global measurement of the time dependence of the gravity field of the planet obtained by the GRACE satellite system. Such data provide a high quality constraint on the dynamic of glacial isostatic adjustment. The code is still under development and the new features we are going to implement comprise:

- the inclusion of the thermal effects, until now only a basic implementation is present, we are evaluating different models and the proper data for obtaining significant results;

- a more detailed model for the Earth, up to now each layer has a constant thickness, in particular the most shallow layers can vary up to an order of magnitude, we are working to include a the depth of the Moho and the topography of the Earth.

References

[1] W. Bangerth, R. Hartmann, and G. Kanschat. deal.II – a general purpose object oriented finite element library. *ACM Trans. Math. Softw.*, 33(4):24/1–24/27, 2007.

[2] Adam M. Dziewonski and Don L. Anderson. Preliminary reference earth model. *Physics of the earth and planetary interiors*, 25(4):297–356, 1981.

[3] A. C. Fowler and Xin-She Yang. Loading and unloading of sedimentary basins: The effect of rheological hysteresis. *Journal of Geophysical Research: Solid Earth*, 107(B4):ETG 1–1–ETG 1–8, 2002.

[4] H. Johansen, W. Fjeldskaar, and J. Mykkeltveit. The influence of glaciation on the basin temperature regime. *Global and Planetary Change*, 12(1–4):437–448, 1996. Impact of Glaciations on Basin Evolution: Data and Models from the Norwegian Margin and Adjacent Areas.

[5] A. Kjemperud and W. Fjeldskaar. Pleistocene glacial isostasy-implications for petroleum geology. *Structural and tectonic modelling and its application to petroleum geology: Norwegian Petroleum Society Special Publication*, 1:187–195, 1992.

[6] W. Richard Peltier. Ice age paleotopography. *Science*, pages 195–201, 1994.

[7] W. Richard Peltier. Mantle viscosity and ice-age ice sheet topography. *Science*, pages 1359–1364, 1996.

[8] W. Richard Peltier. Global glacial isostasy and the surface of the ice-age earth: the ice-5g (vm2) model and grace. *Annu. Rev. Earth Planet. Sci.*, 32:111–149, 2004.

Filling GeoModels with rock physical properties using advanced geostatistical techniques

Didier Renard
Mines ParisTech, PSL Research University
Geosciences Center, 35 rue St Honore 77300 Fontainebleau, France
didier.renard@mines-paristech.fr

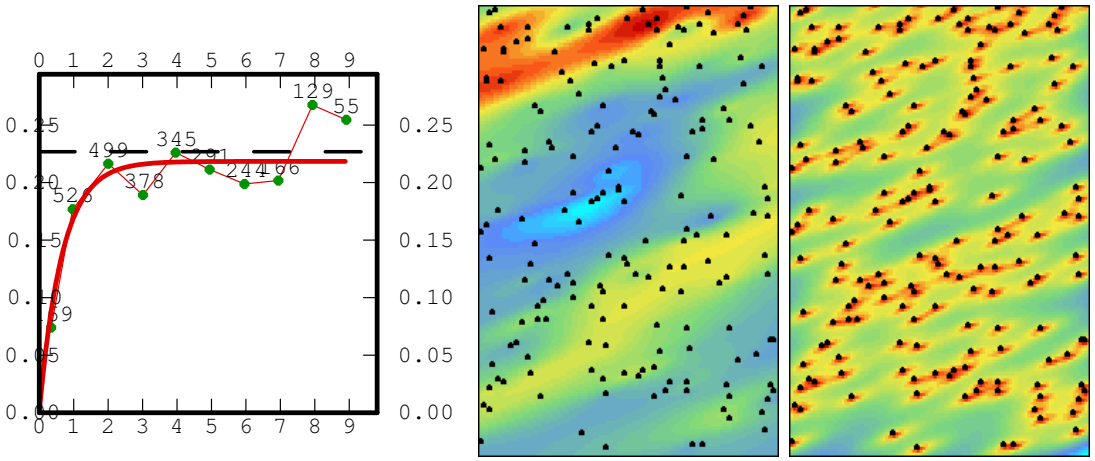
1 Introduction

One of the main challenges of Geostatistics in reservoir characterization is to populate a portion of 3-D earth model with its rock physical properties. This operation must be carried out while still honoring the information available along well logs: in our jargon, we say that it must be conditional. No restriction should be required on this conditioning information, either in number or in its geometry (vertical, deviated or even horizontal wells are allowed). As Geostatistics is taking full advantage of any spatial correlation between variables, it is an essential condition for the data to be transformed into the depositional framework where the horizontal correlation makes sense. This geometrical transformation should be performed beforehand on the well conditioning information. Then we should simply populate a regular working grid of petrophysical parameters which should be brought back to the stratigraphic position ultimately.
The standard geostatistical operations consist in propagating information only known at few conditioning samples onto a large amount of grid nodes or cells, by linearly combining these data. Hence these techniques are limited to variables where linear combinations make sense (additive variables). This is the case for most variables. However let us mention the case of the quantities with a non-linear behavior which must be addressed using specific techniques.

2 Interpolation

The well-known geostatistical technique called *kriging* is a method which performs the interpolation of a given variable, conditioned by some data measured at scattered locations. It produces, in any point in the space (and in particular at the nodes of the regular grid) the most probable interpolated value, constrained by the information. Its prerequisite is narrowed down to the only knowledge of the geostatistical model. We first calculate the experimental *variogram* from the data values which measures its variability as a function of the distance (and orientation). Then this quantity is fitted by a mathematical sound function which describes the spatial continuity and anisotropy of the variable of interest (Figure 1).
Given the variogram model, the kriging procedure interpolates the variable at any target location as a linear combination of the closest data measurements. The set of weights are optimal as they minimize the estimation error which can be expressed using the variogram function. The map of the standard deviation of this estimation error is a by-product of the kriging technique. This technique has been gradually improved in order to account

Figure 1: Experimental Variogram and Fitted Model (left) - Kriging constrained by a set of measurements (black dots): maps of Estimation (middle) and standard deviation of estimation error (right)

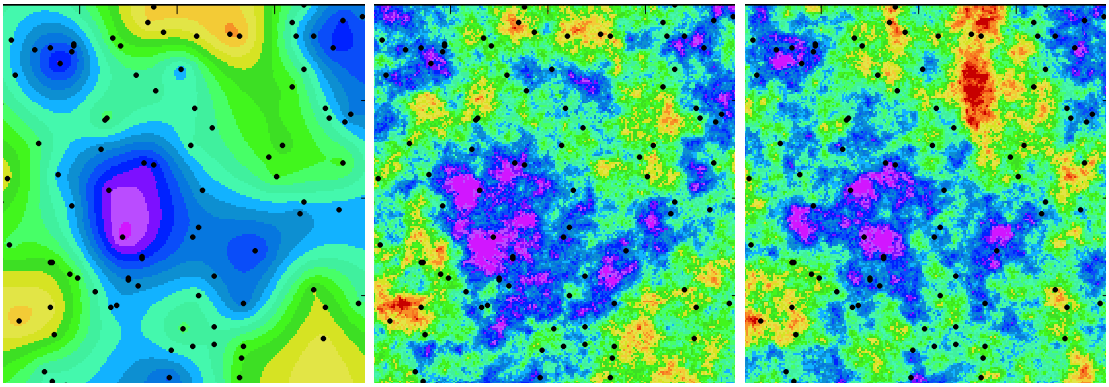


for various properties of the variable, such as the presence of measurement errors, the evidence of a drift in a given direction or any other particularity. Moreover it has been enhanced in order to deal simultaneously with several correlated variables, introducing the *cokriging* technique, where the model involves not only the variograms of each variable but also the cross-variogram of variables considered two by two.
A direct extension of this multivariate technique is the estimation of a main variable informed on few measurements along wells, guided by the knowledge of an auxiliary variable densely sampled (provided by seismic for example). Depending on the nature of the link between the two variables, specific methods have been developed going from the *external drift* algorithm (for a weak dependency where the auxiliary variable only provides the global shape) to the *collocated cokriging* (when the link is established in the model). Finally note that the kriging technique can also cope with the change of support as we often want to estimate the average value of a parameter (say porosity) within a cell whose dimension is by far different from the dimensions of the cores where information is provided. This estimation technique carries a smoothing property inherent to its optimization procedure, although still controlled by the model. This interesting smoothing property is a major drawback when looking for some non-linear characteristics such as the probability that the variable exceeds a threshold.

3 Simulations

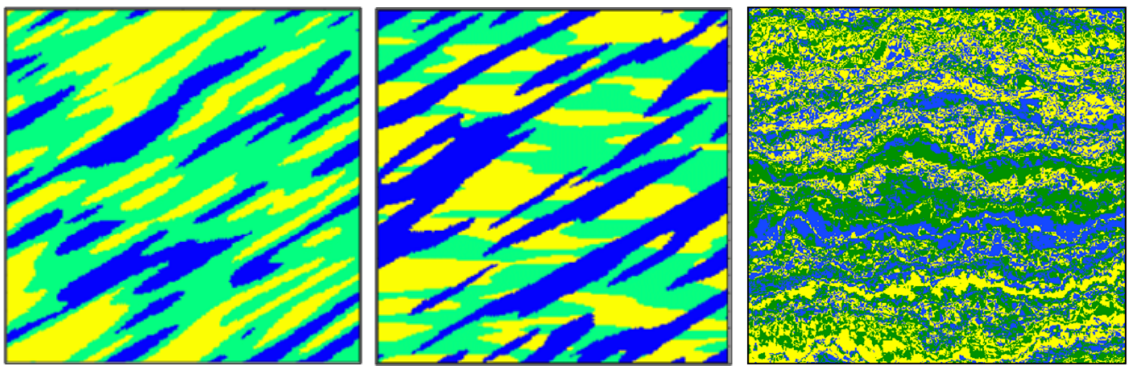
Rather than a smoothed estimation, one may be interested instead by geostatistical *simulations* which reproduce the variability of the variable of interest, as described by the variogram model. This technique produces several plausible scenarios (or outcomes), each one of them being compatible with the data information, hence the name of conditional simulations (Figure 2). Moreover this technique enables to handle the non-linearity behavior of the petrophysical parameters [2]. The basic simulation methodology consists in generating a Gaussian random function (GRF) that honors the variogram model. But a Gaussian simulation fails in reproducing the case where a property experiences abrupt changes in values at short distances, as we move from one lithotype to another in heterogeneous reservoirs. For that reason, the principle consists in simulating lithotype variable first (non numerical but categorical) and then to simulate the petrophysical

Figure 2: Comparing estimation by kriging (left) with two simulations (right)



characteristics per lithotype (using Gaussian simulation for example).
Principal categorical simulation models rely on the truncation of one (TGS) or several (PGS) underlying GRFs; they produce outcomes conditioned by lithotypes measured at wells, honoring their vicinity relationships described in the lithotype rule and following the spatial distribution of their proportions [1][3]. Although PGS can generate complex layouts which cope with most of the sedimentary deposits, the outcomes always present a symmetrical pattern. Specific options have been designed to overcome this symmetry limitation and introduce an orientation in the facies organization [4]. At a smaller scale, the lithotype organization may necessitate to account for characteristics of high frequency transitions (resistivity or rock hardness): the *Substitution* model has been applied [2]. See some outcomes of categorical simulations in Figure 3. The simulation models presented

Figure 3: Categorical Simulations: TGS (left), PGS (middle) and Substitution (right)



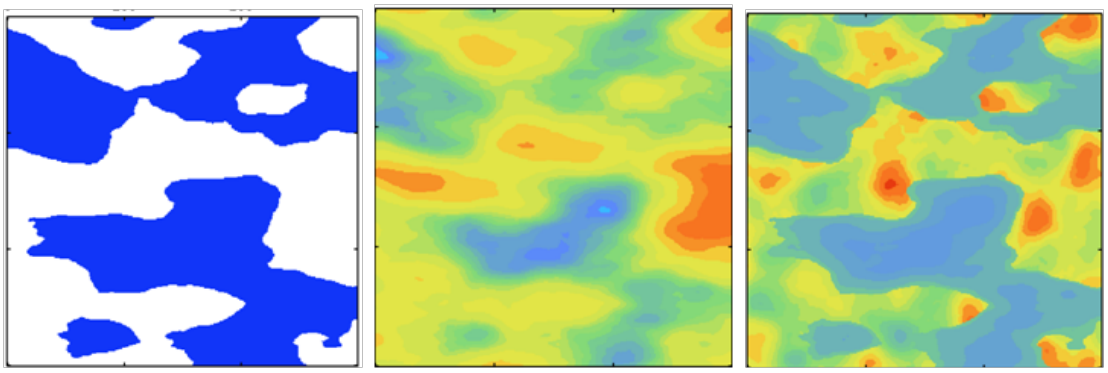
above honor the available data and fulfill the spatial characteristics. However one may think of additional constraints on the lithotype simulation part (lithotype connectivity) or on the way the different lithotypes are filled afterwards with rock properties (inequalities, edge effect when changing lithotype as in Figure 4)

References

[1] Armstrong, M., Galli, A., Beucher, H., Le Loc'h, G., Renard, D., Doligez, B., Eschard, R. and Geffroy, F. 2011 *Plurigaussian Simulations in Geosciences.* 2nd ed. Springer, Berlin, Germany.

[2] Lantuéjoul, C. 2001 *Geostatistical simulation: models and algorithms.* Springer, Berlin.

Figure 4: Categorical Simulation (left) - Filling with (middle) and without (right) edge effect



[3] Matheron, G., Beucher, H., de Fouquet, C., Galli, A., Guérillot, D. and Ravenne, C. 1987 *Conditional Simulation of the Geometry of Fluvio-Deltaic Reservoirs*, SPE 16753

[4] Renard, D. and Beucher, H. 2012 *3-D representations of a uranium roll-front deposit.* Institute of Materials, Minerals and Mining - AusIMM.

Erosion, sedimentation, landscape evolution, and interaction with tectonics & geodynamics – coupled numerical models

Kosuke Ueda
Department of Earth Sciences, ETH Zürich
Sonneggstrasse 5, 8092 Zürich Switzerland
kosuke.ueda@erdw.ethz.ch

Taras Gerya
Department of Earth Sciences, ETH Zürich
Sonneggstrasse 5, 8092 Zürich Switzerland
taras.gerya@erdw.ethz.ch

Sean Willett
Department of Earth Sciences, ETH Zürich
Sonneggstrasse 5, 8092 Zürich Switzerland
swillett@ethz.ch

Basin development aligns a geodynamic creation of accommodation, tectonic provision of relief, and surface-bound source erosion, transport, and deposition of available supply. Deformation and surface process interact on local and regional scale in redistributing mass and stresses. An economically relevant basin history is further characterized by thermal evolution, developing overburden, and associated changes in rock properties and potential pathways.

In numerical approaches, linking model and data parameters forward, various challenges exist in combining discretized and sometimes parametrized physical descriptions of geological processes across time and depth scales. Available tools are often specialized, and suited to either capture the lithospheric-scale creation of accommodation, regional strain partitioning, and thermal evolution (geodynamic / thermomechanical models), or successfull in modelling landscape evolution, surface processes, and basin fill (landscape evolution models, LEM).

We present and assess recent developments in coupling different discretizations of the surface in two LEM, with a thermomechanical finite-difference model in three dimensions. We apply a fluvial LEM to study tectonics-surface process interaction in accretionary wedges, where we also demonstrate the sensitivity to lithological erosion feedback and regional precipitation; demonstrate characteristic response of a fluvial LEM in a geodynamic collision model; show proof-of-concept for continental break-up and rift formation; and highlight a surface process influence on upper-mantle scale plate models.

These type of modelling approaches account, in principle, sufficiently well for mechanical and thermal complexity as well as surface mass redistribution, and are potentially suitable to extract geologically comparable synthetic observables, such as lithology, stratigraphy, thermochronology, or vitrinite reflectance records.

New Mathematical Trends in Imaging - Part I

PROPOSERS

Alessandro Lanza
Dip. Matematica, Università degli Studi di Bologna
P.zza Porta San Donato, 5 - Bologna Italy
alessandro.lanza2@unibo.it

Serena Morigi
Dip. Matematica, Università degli Studi di Bologna
P.zza Porta San Donato, 5 - Bologna Italy
serena.morigi@unibo.it

SPEAKERS

Alessandro Foi (keynote)
Dept. of Signal Processing, Tampere University of Technology, Tampere, Finland
alessandro.foi@tut.fi

Stefania Bellavia
Dip. di Ingegneria Industriale, Università di Firenze
stefania.bellavia@unifi.it

Claudio Estatico
Dip. di Matematica, Università di Genova
estatico@dima.unige.it

Federica Porta
Dip. di Matematica e Informatica, Università di Ferrara
federica.porta87@gmail.com

Simone Rebegoldi
Dip. di Scienze Fisiche, Informatiche e Matematiche, Università di Modena e Reggio Emilia
simone.rebegoldi@unimore.it

The aim of this minisymposium is to bring together researchers in various aspects of mathematical image processing to share the latest developments in this field and to leverage the synergy between accademic research and real applicative interests in image processing. The minisymposium will cover two parts: the first is dedicated to mathematical developments in imaging focusing on variational models and emerging related optimization techniques; the second part is devoted to investigate several aspects of imaging science ranging from hardware design to image enhancement, from image representation to image understanding, from the point of view of experts working in the field. Variational models are getting popular for image processing and other imaging problems including inverse problems, image reconstruction and computer vision. The search for fast and robust algorithms to solve variational models, however, is an open challenge to the mathematical community due to complexity involved with: nonlinearity, non-smoothness of functional and solutions, non-convexity for the minimization, high-order derivatives within the functional, and large data size. Both the use of advanced optimization techniques and

the development of new techniques are of fundamental importance for the success of elaborations in different imaging applications. This motivates this proposal to bring researchers from industrial and mathematical community to exchange and stimulate ideas in imaging sciences, to combine deep theoretical contributions with very relevant emerging practical applications.

Efficient restoration of extremely low count Poisson Images using off-the-shelf Gaussian filters

Alessandro Foi
Tampere University of Technology
P.O. Box 553, FIN-33101 Tampere, Finland
alessandro.foi@tut.fi

Poisson noise is characteristic of many image acquisition modalities and its removal is of fundamental importance for many applications, particularly in astronomy and biomedical imaging. As the noise variance equals the expected value of the underlying true signal, Poisson noise is signal dependent, which makes the premise for Poisson image restoration very different from the case of additive white Gaussian noise with constant variance typically assumed by common signal processing filters. Variance-stabilizing transformations (VST) (*e.g.*, [1]) are nonlinear mappings which are commonly employed in order to reduce a signal corrupted by signal-dependent noise to a signal where the noise variance is constant and that can be thus processed by common filters.

In this talk we will review the VST approach, from its fundamentals [4, 5, 3] to its most recent advances [6, 7, 9, 8], emphasizing the benefits and the intrinsic limitations of this classical method which has been the workhorse of Poisson data processing for nearly a century. We conclude by introducing an iterative framework for progressively improving the effectiveness of VST through iterated combinations of the Poisson observations with the filtered estimate from the previous iteration [2]. This results in a very fast and stable algorithm that yields significantly better quality, particularly at low and extremely low SNR (e.g., less than a count per pixel), outperforming much costlier state-of-the-art alternatives.

References

[1] Anscombe, F.J., "The transformation of Poisson, binomial and negative-binomial data", *Biometrika*, vol. 35, no. 3/4, pp. 246–254, Dec. 1948.

[2] Azzari, L. and Foi, A., "Variance Stabilization for Noisy+Estimate Combination in Iterative Poisson Denoising", submitted to *IEEE Signal Processing Letters*, 2016.

[3] Bar-Lev, S. K., and P. Enis, "On the construction of classes of variance stabilizing transformations", *Statistics & Probability Letter* , vol. 10, pp. 95–100, July 1990.

[4] Curtiss, J.H., "On transformations used in the analysis of variance", *The Annals of Mathematical Statistics*, vol. 14, no. 2, pp. 107–122, June 1943.

[5] Efron, B., "Transformation theory: How normal is a family of distributions?", *The Annals of Statistics*, vol. 10, no. 2, pp. 323–339, 1982.

[6] Foi, A., "Clipped noisy images: heteroskedastic modeling and practical denoising", *Signal Processing*, vol. 89, no. 12, pp. 2609-2629, December 2009.

[7] Foi, A., "Direct optimization of nonparametric variance-stabilizing transformations", presented at *èmes Rencontres de Statistiques Mathématiques*, CIRM, Luminy, France, December 2008.

[8] Foi, A., "Noise estimation and removal in MR imaging: the variance-stabilization approach", *Proceedings of the 2011 IEEE International Symposium on Biomedical Imaging (ISBI 2011)*, Chicago, IL, USA, 30 March - 2 April 2011.

[9] Mäkitalo, M., and A. Foi, "Optimal inversion of the Anscombe transformation in low-count Poisson image denoising", *IEEE Transactions on Image Processing*, vol. 20, no. 1, pp. 99–109, January 2011.

Regularized quadratic penalty methods for shape from shading

Stefania Bellavia
Università degli Studi di Firenze
Dipartimento di Ingegneria Industriale, viale G.B. Morgagni 40, 50134 Firenze, Italia
stefania.bellavia@unifi.it

Lapo Governi
Università degli Studi di Firenze
Dipartimento di Ingegneria Industriale, via di S.Marta 3, 50139 Firenze, Italia
lapo.governi@unifi.it

Alessandra Papini
Università degli Studi di Firenze
Dipartimento di Ingegneria Industriale, viale G.B. Morgagni 40, 50134 Firenze, Italia
benedetta.morini@unifi.it

Luca Puggelli
Università degli Studi di Firenze
Dipartimento di Ingegneria Industriale, via di S.Marta 3, 50139 Firenze, Italia
luca.puggelli@unifi.it

Shape from shading (SFS) denotes the problem of reconstructing a 3D surface, starting from a single shaded image which represents the surface itself. Minimization techniques are commonly used for solving the SFS problem, where the objective function is a weighted combination of the brightness error, plus one or more terms aiming to obtain a valid solution. The possibility of obtaining a good reconstruction largely depends on the nontrivial choice of the weights, also because in practice the sought exact solution rarely happens to minimize the used model. We present a regularized quadratic penalty method where quadratic penalization is used to adaptively adjust the smoothing weights, so that an a-priori choice is not needed. Further, a suitable quadratic regularization term is added to improve the robustness and reliability of the procedure. In fact, the SFS problem is replaced by a sequence of unconstrained subproblems, which are efficiently solved by a nonmonotone Barzilai-Borwein method. Numerical results are provided showing the reliability of the proposed approach.

Delta-convex minimization and variable exponent Lebesgue spaces for imaging

Claudio Estatico
Università degli Studi di Genova, Dipartimento di Matematica
via Dodecaneso, 35 16136 - Genova, Italy
estatico@dima.unige.it

Fabio Di Benedetto
Università degli Studi di Genova, Dipartimento di Matematica
via Dodecaneso, 35 16136 - Genova, Italy
dibenede@dima.unige.it

Flavia Lenti
Institut de Recherche en Informatique de Toulouse, ENSEEIHT
2 Rue Charles Camichel, F-31000 Toulouse, France
lenti@cerfacs.fr

We consider the solution of the linear functional equation $Ax = y$ arising in image restorations, characterized by an ill-posed operator $A : X \longrightarrow Y$ between two complete normed linear functional spaces X and Y. The conventional variational approach involves the minimization of a Tikhonov-type regularization functional $\Phi_\alpha : X \longrightarrow \mathbb{R}$ defined as

$$\Phi_\alpha(x) = \mathcal{D}(Ax, y) + \alpha\mathcal{R}(x)\,.$$

The functional Φ_α is the sum of a data fitting functional $\mathcal{D} : Y \times Y \longrightarrow \mathbb{R}$ which measures some distance between Ax and y, and a convex regularization term $\mathcal{R} : X \longrightarrow \mathbb{R}$ which quantifies the "non-regularity" of x [5], whereas the regularization parameter $\alpha > 0$ balances between data fitting and stability.

In the simplest case, referred as (basic) Tikhonov regularization, both X and Y are Hilbert spaces, $\mathcal{D}(Ax, y) = \frac{1}{2}\|Ax - y\|_Y^2$ and $\mathcal{R}(x) = \frac{1}{2}\|x\|_X^2$. In the last two decades, several other choices for the residual functional $\mathcal{D}$ and the penalty functional $\mathcal{R}$ have been proposed in the literature to reduce the over-smoothness effects of the basic Hilbertian Tikhonov solutions x_α, also aimed at improving the sparsity, or at enforcing non-negativity or other special constraints. We just mention a few, such as special weighted norms $\mathcal{D}(Ax, y) = p^{-1}\|Ax - y\|_p^p$ in Lebesgue spaces L^p or in Sobolev spaces $W^{k,p}$, for $1 < p < +\infty$, and $\mathcal{R}(x) = q^{-1}\|x\|_q^q$, or $\mathcal{R}(x) = q^{-1}\|Lx\|_q^q$ for some special penalty operators L, such as differential operators, for $1 < q = p^* < +\infty$. Other popular choices are related to the total variation approach, or to fixed reference approximations properly selected to attain sparsity [6].

In this talk, we first introduce a special Tikhonov-type functional Φ_α whose penalty term $\mathcal{R}$ is model-dependent, that is, differing from the classical proposals, $\mathcal{R}$ explicitly depends on the operator A which characterizes the functional equation [3]. In addition, the functional is no longer convex as in the conventional setting, but in our proposal is delta-convex; i.e., it is representable as a difference of two convex terms.

We will show that the proposed delta-convex functional allows us to speed up the convergence of iterative gradient minimization algorithms (naturally possessing a regularization effect), since the second term to be subtracted in the functional plays a new role, aiming to accelerate the iterations; therefore the related coefficient now balances between regularization and speed-up, and must take larger values in the very early iterations. This acceleration technique, which we call as "irregularization", is useful for large scale equations arising in image restoration [1].

Finally, an extension of the Tikhonov regularization to the unconventional variable exponent Lebesgue space $L^{p(\cdot)}$ is analyzed and numerically tested, aimed at providing a pointwise and adaptive control of the level of regularization. More specifically, a variable exponent Lebesgue space $L^{p(\cdot)}$ is a Lebesgue space where the exponent $p \geq 1$ used for the definition of the norm is not constant, but rather it is pointwise variable as a function $p(\cdot)$ of the domain [2]. Such a functional space $L^{p(\cdot)}$ is used to obtain, in the same restoration process, different levels of regularization between the areas where the true object is located and the areas where only the background is present. The proposal represents a natural and continuous extension of early procedures previously based on image segmentation, developed to vary the level of regularization depending on the "local" signal to noise ratios in the different portions of the image do main [4].

References

[1] Brianzi P., Di Benedetto F., Estatico, C., and Surace, L. 2016 *Irregularization accelerates iterative regularization.* Submitted.

[2] Diening, L., Harjulehto, P., Hästö, P., Ruzicka, M. 2011 *Lebesgue and Sobolev spaces with variable exponents.* Lecture Notes in Mathematics. vol. 2017.

[3] Huckle, T, and Sedlacek M. 2012 *Tykhonov-Phillips regularization with operator dependent seminorm.* Numer. Alg., vol. 60, pp. 339–353.

[4] Nagy J. C., Pauca P., Plemmons, R. J., and Torgersen, T.C. 1997 *Space-Varying Restoration of Optical Images.* J. Optic. Soc. Amer. A, vol. 14, 3162–3174.

[5] Scherzer, M.O., Grasmair, M., Grossauer, H., Haltmeier, M., and Lenzen, F. 2009 *Variational Methods in Imaging.* Springer, Berlin.

[6] Schuster, T., Kaltenbacher, B., Hofmann, B., and Kazimierski, K. S. 2012 *Regularization Methods in Banach Spaces.* Radon Series on Computational and Applied Mathematics, vol. 10, De Gruyter.

A variable metric proximal-gradient method with extrapolation

Federica Porta
Università di Ferrara
via Saragat, 1 44100 - Ferrara Italy
federica.porta@unife.it

Silvia Bonettini
Università di Ferrara
via Saragat, 1 44100 - Ferrara Italy
silvia.bonettini@unife.it

Valeria Ruggiero
Università di Ferrara
via Saragat, 1 44100 - Ferrara Italy
valeria.ruggiero@unife.it

In this work we consider the optimization problem

$$\min_{\boldsymbol{x}\in\mathbb{R}^n} F(\boldsymbol{x}) \equiv f(\boldsymbol{x}) + g(\boldsymbol{x}) \tag{1}$$

where f and g are two proper convex and lower semicontinuous functions from $\mathbb{R}^n$ to $\mathbb{R}\cup\{\infty\}$. Moreover, we also assume that f is differentiable with Lipschitz continuous gradient on a suitable closed, convex set $Y \subseteq \mathrm{dom}(f) = \{x \in \mathbb{R}^n : f(x) < +\infty\}$.
Model (1) allows to formalize several problems arising from real-life applications such as signal and image processing, statistical inference and machine learning. A typical feature of these applications is the large number of variables, which makes the class of first order methods very attractive. In this class, forward-backward methods [10, 7] are especially suited for problem (1), since they exploit the decomposition of the objective function in a differentiable term and a nondifferentiable one. The general forward-backward iteration is given by

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + \lambda_k(\mathrm{prox}_{\alpha_k g}(\boldsymbol{x}^{(k)} - \alpha_k \nabla f(\boldsymbol{x}^{(k)})) - \boldsymbol{x}^{(k)}), \tag{2}$$

where λ_k, α_k are positive parameters controlling the steplength and $\mathrm{prox}_{\phi}(\cdot)$ is the proximity operator associated to the convex function ϕ, which is defined as

$$\mathrm{prox}_{\phi}(\boldsymbol{y}) = \operatorname*{argmin}_{\boldsymbol{x}\in\mathbb{R}^n} \ \phi(\boldsymbol{x}) + \frac{1}{2}\|\boldsymbol{x}-\boldsymbol{y}\|^2 \tag{3}$$

Forward-backward methods are easy to implement and have well studied convergence properties. On the other hand, it is well known that they can exhibit a poor convergence rate, especially when a high accuracy is required. In the recent literature we can find two different approaches aiming to improve the convergence speed of forward-backward methods. They are both described below.

Inertial/extrapolation techniques This approach consists in adding an extrapolation step to the basic forward-backward iteration, yielding a multistep algorithm. The idea of inertial methods becomes very popular in the last decade, in view of Nesterov's work [11] and it has been further developed in [1], where the authors propose the following variant

$$\begin{aligned} \boldsymbol{y}^{(k)} &= \boldsymbol{x}^{(k)} + \beta_k(\boldsymbol{x}^{(k)} - \boldsymbol{x}^{(k-1)}) && (4)\\ \boldsymbol{x}^{(k+1)} &= \mathrm{prox}_{\alpha_k g}(\boldsymbol{y}^{(k)} - \alpha_k \nabla f(\boldsymbol{y}^{(k)}))\,. && (5) \end{aligned}$$

In [1, 2], the convergence of method (4)–(5) is investigated by showing that for suitable sequences of parameters $\{\alpha_k\}$ and $\{\beta_k\}$ (with $\lim_k \beta_k = 1$) one has an $\mathcal{O}\left(\frac{1}{k^2}\right)$ convergence rate estimate on the objective function values.
The main limitations on the use of method (4)–(5) are that it may be unfeasible when $\mathrm{dom}(f)$ does not coincide with the whole space $\mathbb{R}^n$ and that the convergence of the iterates $\{\boldsymbol{x}^{(k)}\}$ is guaranteed only under more restrictive assumptions [6].

Variable metric/scaling techniques In a variable metric forward-backward algorithm the underlaying metric may change at each iteration by means of suitable symmetric positive definite scaling matrices multiplying the gradient of f and also involved in the definition of the proximity operator. The expected advantage in using a variable metric is an improved capability to capture the local features of problem (1), possibly leading to an improvement of the convergence speed. In [8, 9], the authors propose the following variable metric forward-backward algorithm

$$\boldsymbol{x}^{(k+1)} = \boldsymbol{x}^{(k)} + \lambda_k(\mathrm{prox}^{D_k}_{\alpha_k g}(\boldsymbol{x}^{(k)} - \alpha_k D_k \nabla f(\boldsymbol{x}^{(k)})) - \boldsymbol{x}^{(k)})\,, \qquad (6)$$

where $\{D_k\}$ is a sequence of symmetric positive definite matrices and $\mathrm{prox}^{D_k}_{\alpha_k g}(\boldsymbol{y})$ is defined as

$$\mathrm{prox}_{\phi}(\boldsymbol{y}) = \underset{\boldsymbol{x}\in\mathbb{R}^n}{\mathrm{argmin}}\ \ g(\boldsymbol{x}) + \frac{1}{2\alpha_k}(\boldsymbol{x}-\boldsymbol{y})D_k^{-1}(\boldsymbol{x}-\boldsymbol{y})\,. \qquad (7)$$

Method (6), equipped by an Armijo line–search for the computation of λ_k, has been extensively studied in the papers [3, 4, 5] when $g(x)$ reduces the indicator function of a closed convex subset of $\mathbb{R}^n$. The convergence rate on the objective function values in this case is only linear (see [4]). However, in spite of the theoretical convergence rate, a suitable combination of the stepsize parameter α_k and the scaling matrix D_k can allow the method (6) to reach practical performances which are comparable with those of (4)–(5) [4, 12].
In this work we combine the two acceleration techniques described above and we propose a variable metric proximal-gradient method with extrapolation. In particular we address the case where $\mathrm{dom}(f)$ is a proper subset of $\mathbb{R}^n$ and we devise an implementable condition on the sequence $\{D_k\}$ to ensure both the convergence of the iterates sequence $\{\boldsymbol{x}^{(k)}\}$ and the $\mathcal{O}\left(\frac{1}{k^2}\right)$ convergence rate of the objective function values. The effectiveness of the proposed method is evaluated by means of a comparison with other state-of-the-art algorithms, on several optimization problems of the form (1), arising from different real-life applications such as image deblurring, compressed sensing, and probability density estimation.

References

[1] A. Beck and M. Teboulle. A fast iterative shrinkage-thresholding algorithm for linear inverse problems. *SIAM J. Imaging Sci.*, 2:183–202, 2009.

[2] D. Bertsekas. *Convex Optimization Theory*, chapter 6 on Convex Optimization Algorithms, pages 251–489. 5 november 2012 edition.

[3] E. G. Birgin, J. M. Martinez, and M. Raydan. Inexact spectral projected gradient methods on convex sets. *IMA J. Numer. Anal.*, 23(4):539–559, October 2003.

[4] S. Bonettini and M. Prato. New convergence results for the scaled gradient projection method. *Inverse Problems*, 31(9):095008, 2015.

[5] S. Bonettini, R. Zanella, and L. Zanni. A scaled gradient projection method for constrained image deblurring. *Inverse Probl.*, 25(1):015002, January 2009.

[6] A. Chambolle and C. Dossal. On the convergence of the iterates of "FISTA". September 2014.

[7] P.L. Combettes and J.-C. Pesquet. Proximal splitting methods in signal processing. In H. H. Bauschke, R. S. Burachik, P. L. Combettes, V. Elser, D. R. Luke, and H. Wolkowicz, editors, *Fixed-point algorithms for inverse problems in science and engineering*, Springer Optimization and Its Applications, pages 185–212. Springer, New York NY, 2011.

[8] P.L. Combettes and B.C. Vũ. Variable metric quasi-Féjer monotonicity. *Nonlinear Analysis: Theory, Methods, and Applications*, 78:17–31, feb 2013.

[9] P.L. Combettes and B.C. Vũ. Variable metric forward-backward splitting with applications to monotone inclusions in duality. *Optimization*, 63(9):1289–1318, 2014.

[10] P.L. Combettes and V. R. Wajs. Signal recovery by proximal forward-backward splitting. *Multiscale Modeling & Simulation*, 4(4):1168–1200, 2005.

[11] Yu. Nesterov. Smooth minimization of non-smooth functions. *Math. Program.*, 103(1):127–152, 2005.

[12] F. Porta, M. Prato, and L. Zanni. A new steplength selection for scaled gradient methods with application to image deblurring. *Journal of Scientific Computing*, in press, 2015.

Accelerated gradient-based methods for phase estimation in differential-interference-contrast microscopy

Simone Rebegoldi
Università di Modena e Reggio Emilia
Via Campi 213/B, 41125 Modena, Italy
simone.rebegoldi@unimore.it

Lola Bautista
Universidad Industrial de Santander
680002 Bucaramanga, Colombia
bautista@i3s.unice.fr

Laure Blanc-Féraud
Université Nice Sophia Antipolis
06903 Sophia Antipolis, France
laure.blanc_feraud@inria.fr

Marco Prato
Università di Modena e Reggio Emilia
Via Campi 213/B, Modena, Italy
marco.prato@unimore.it

Luca Zanni
Università di Modena e Reggio Emilia
Via Campi 213/B, Modena, Italy
luca.zanni@unimore.it

Arturo Plata
Universidad Industrial de Santander
680002 Bucaramanga, Colombia
aplatag@yahoo.com

In the last forty years, differential-interference-contrast (DIC) microscopy has gained popularity in biomedical research as an effective optical microscopy technique used to observe unstained transparent specimens under a transmitted-light configuration. The DIC image formation is caused by the interference of two orthogonally polarized beams, which are laterally split of a few tenths of a micrometer by a Wollaston prism, phase shifted when passing through different materials across the specimen and then successively recombined by a sliding prism. The resulting image has a three dimensional, high contrast appearance, which can be enhanced by adjusting the sliding prism along the direction of the split in order to introduce a uniform phase difference between the two beams.
From the mathematical viewpoint, the DIC image acquisition is described by the following

nonlinear model [1, 5]

$$o_{k,\lambda} = \left| h_{k,\lambda} * e^{-i\frac{\phi}{\lambda}} \right|^2 + \eta_k, \tag{1}$$

where $\phi \in \mathbb{R}^n$ is the true phase function, k is the rotation index and λ is the value of the RGB wavelength in micrometers, $o_{k,\lambda} \in \mathbb{R}^n$ and $h_{k,\lambda} \in \mathbb{C}^n$ are respectively the observed image and the DIC Point-Spread-Function at the $k-$th rotation of the specimen and illumination wavelength λ, $*$ is the convolution operator, $|\cdot|^2$ is the component-wise square modulus and η_k is the realization of a Gaussian random variable with zero mean and variance σ^2. Following the rotational-diversity model proposed in [5] and furtherly extended in [1], one is interested in retrieving the specimen's phase function from a set of DIC intensity images acquired at different rotations of the specimen. Since this problem is highly ill-posed, one must look for a solution of the following regularized minimization problem

$$\min_{\phi \in \mathbb{R}^n} J_{LS}(\phi; o) + J_R(\phi), \tag{2}$$

where J_{LS} is a least-squares term measuring the distance between the observed image $o_{k,\lambda}$ and the predicted image and J_R is the regularization term.
When a differentiable regularizer, such as a Tikhonov penalty term, is considered, one can address (2) by means of a nonlinear conjugate gradient method [5], which is particularly suited for least squares problems. However, the computation of the line search parameter at each iteration may require several evaluations of both the function and its gradient in order to ensure convergence [4], which significantly increases computational time when such evaluations are expensive, as is the case of the DIC functional. Furthermore, a conjugate gradient method can not handle the presence of a non differentiable regularizer, such as the total variational functional.
To overcome these limits, we propose to address the problem of phase estimation in DIC microscopy by means of a recently proposed proximal-gradient method [2]. The key features of this approach are the use of an Armijo–like rule to determine the step size along the descent direction and the possibility of adopting a variable metric to compute the proximal point. Since providing an efficient scaling matrix for the DIC problem is a quite difficult task, the acceleration of the method relies uniquely on a clever adaptive choice of the stepsize at each iteration [3]. The method is shown to be efficient both when the total variational functional and a smooth approximation of it is used. In the latter case, the method shows also significant improvements in terms of efficiency and stability with respect to widely used conjugate gradient methods.

References

[1] Bautista L., Rebegoldi S., Blanc-Féraud L., Prato M., Zanni L., Plata A. (2016) Phase estimation in differential-interference-contrast (DIC) microscopy. IEEE Proceedings of the 12th International Symposium on Biomedical Imaging, in press.

[2] Bonettini S., Loris I., Porta F., Prato M. (2016) Variable metric inexact line–search based methods for nonsmooth optimization. SIAM Journal on Optimization, Vol. 26, pp. 891–921.

[3] Fletcher R. (2012) A limited memory steepest descent method. Mathematical Programming, Vol. 135, No. 1–2, pp. 413–436.

[4] Gilbert J. C., Nocedal. J. (1992) Global convergence properties of conjugate gradient methods for optimization. SIAM Journal on Optimization, Vol. 2, No. 1, pp. 21–42.

[5] Preza C. (2000) Rotational-diversity phase estimation from differential interference contrast microscopy images. Journal of the Optical Society of America A, Vol. 17, No. 3, pp. 415–424.

New Mathematical Trends in Imaging - Part II

PROPOSERS

Alessandro Lanza
Dip. Matematica, Università degli Studi di Bologna
P.zza Porta San Donato, 5 - Bologna Italy
alessandro.lanza2@unibo.it

Serena Morigi
Dip. Matematica, Università degli Studi di Bologna
P.zza Porta San Donato, 5 - Bologna Italy
serena.morigi@unibo.it

SPEAKERS

Maurizio De Girolami
Datalogic, Bologna
Maurizio.DeGirolami@datalogic.com

Alessandro Lanza
Dip. di Matematica, Università di Bologna, Bologna
alessandro.lanza2@unibo.it

Anna Maria Massone
CNR - SPIN, Genova
annamaria.massone@cnr.it

Patrizia Melpignano
OR-EL.doo at Primorski Tehnoloski Park, Slovenija
melpypat@gmail.com

Giuseppe Rodriguez
Dip. di Matematica e Informatica - Università di Cagliari
rodriguez@unica.it

The aim of this minisymposium is to bring together researchers in various aspects of mathematical image processing to share the latest developments in this field and to leverage the synergy between accademic research and real applicative interests in image processing. The minisymposium will cover two parts: the first is dedicated to mathematical developments in imaging focusing on variational models and emerging related optimization techniques; the second part is devoted to investigate several aspects of imaging science ranging from hardware design to image enhancement, from image representation to image understanding, from the point of view of experts working in the field. Variational models are getting popular for image processing and other imaging problems including inverse problems, image reconstruction and computer vision. The search for fast and robust algorithms to solve variational models, however, is an open challenge to the mathematical community due to complexity involved with: nonlinearity, non-smoothness of functional and solutions, non-convexity for the minimization, high-order derivatives within the functional, and large data size. Both the use of advanced optimization techniques and

the development of new techniques are of fundamental importance for the success of elaborations in different imaging applications. This motivates this proposal to bring researchers from industrial and mathematical community to exchange and stimulate ideas in imaging sciences, to combine deep theoretical contributions with very relevant emerging practical applications.

Automatic Barcode Reading: Problem Definition, State-of-the-art and Some Open Problems

Maurizio De Girolami
Datalogic IP Tech S.r.l.
Via San Vitalino 13, 40012 - Lippo di Calderara di Reno, Bologna, Italy
Maurizio.DeGirolami@datalogic.com

Francesco Deppieri
Datalogic IP Tech S.r.l.
Via San Vitalino 13, 40012 - Lippo di Calderara di Reno, Bologna, Italy
Francesco.Deppieri@datalogic.com

The process of automatic barcode reading and decoding is of great importance in many application fields, namely any field where a request for automatic recognition and identification of objects and/or persons arises. The possible applications are indeed very varied and range from the commercial (retail application) to the industrial (warehouse management, identification of items in postal and airport applications), safety (automatic access control) and mobile devices (automatic link) field, thus rendering barcode decoding a ubiquitous process in many aspects of people's everyday life.
A crucial requirement for barcode reading algorithms is real-time processing with fast response time (on the order of tenths of a second), also on cheap, poorly performing hardware. Moreover, due to the great variability of possible application conditions, robustness against potential distortions of the processed signals, such as noise, blur, poor illumination, low resolution, print errors, is a desirable property. In fact, the higher this robustness, the wider the range of working conditions under which a reliable barcode decoding can be obtained (for instance, higher admissible distance between barcode and sensing system, lower resolution and lower quality of the optics of the sensing system), this holding the potential for positive impacts also in economic terms.
Beyond certain levels of distortion of the processed signals, performance of traditional numerical methodologies for barcode decoding, based on detection/elaboration of local features such as signal fronts, inflection points and extrema, rapidly decreases. Hence arises the necessity for alternative decoding paradigms, i.e. for novel and more performing mathematical/numerical models/methods.
In this talk, first the problem of automatic barcode decoding will be framed from the applicative point of view: the most important application fields will be illustrated together with the most diffused barcode types (symbologies) and the different technologies used for sensing the data (signals/images) by which decoding is carried out. Then, a mathematical/statistical formulation of the barcode decoding problem will be given and today's most diffused algorithmic paradigms will be outlined while at the same time highlighting their strengths and, more interestingly, their weaknesses. Finally, the last part of this contribution will be devoted to briefly outlining some important and, to some extent, open mathematical/numerical problems for the industrial barcode reading community. In fact, a rigorous mathematical/numerical approach holds the potential for fruitfully contributing to device more effective and, maybe, more efficient solutions.

Convex Image Denoising via Non-convex Regularization with Automatic Parameters Selection

Alessandro Lanza
University of Bologna - Department of Mathematics
Piazza di Porta S. Donato 5, 40126 - Bologna, Italy
alessandro.lanza2@unibo.it

Serena Morigi
University of Bologna - Department of Mathematics
Piazza di Porta S. Donato 5, 40126 - Bologna, Italy
serena.morigi@unibo.it

Fiorella Sgallari
University of Bologna - Department of Mathematics
Piazza di Porta S. Donato 5, 40126 - Bologna, Italy
fiorella.sgallari@unibo.it

Noise is an unavoidable component of digital image acquisition, and as such, noise removal is a fundamental task in digital image processing. The challenge is to preserve and possibly enhance important image features during the denoising process, such as edges, corners, textures and fine details. One of the most ubiquitous and, hence, most studied noise types is the Additive White Gaussian Noise (AWGN), which corrupts all image pixels by independent and identically distributed Gaussian disturbs.
We present a novel Convex Non-Convex (CNC) denoising variational model for restoring images corrupted by AWGN. In particular, we propose the use of parameterized non-convex regularization terms to effectively induce sparsity of the gradient magnitudes in the solution, while maintaining strict convexity of the total cost functional. Some widely used non-convex regularization functions are evaluated and a new one is analyzed which allows for better restorations. An efficient minimization algorithm based on the Alternating Directions Methods of Multipliers (ADMM) strategy is proposed for simultaneously restoring the image and automatically selecting the regularization parameter by exploiting the discrepancy principle. Theoretical convexity conditions for both the proposed CNC variational model and the optimization sub-problems arising in the ADMM-based procedure are provided which guarantee convergence to a unique global minimizer. Numerical examples are presented which indicate how the proposed approach is particularly effective and well suited for images characterized by moderately sparse gradients.

An extension of the Hough transform with effective applications in medical imaging

Anna Maria Massone
CNR - SPIN
via Dodecaneso, 33 16146 - Genova Italy
annamaria.massone@cnr.it

Cristina Campi
Università degli Studi di Roma 'La Sapienza'
via A. Scarpa 14, 00161 Roma Italy
cristina.campi@sbai.uniroma1.it

Mauro C. Beltrametti
Università degli Studi di Genova
via Dodecaneso, 35 16146 - Genova Italy
beltrametti@dima.unige.it

The Hough transform is a classical pattern recognition technique employed to extract straight lines [3], circles and ellipses [2] in images. Recently, algebraic geometry arguments have been proposed [1] in order to apply the Hough transform framework to special families $\mathcal{F}$ of irreducible algebraic plane curves that share the degree; first applications to medical and astronomical images have been presented in [4].
The idea at the basis of this approach is that points lying on a curve in the image space can be transformed into hypersurfaces (their Hough transforms) in the parameter space, and the set of parameters corresponding to the intersection of all Hough transforms identifies the curve to be recognized in the image space. The goal of this talk is to show how the set of parameters characterizing the detected curves can be effectively used to infer significant information from medical images in the case of hematological malignancies, such as Advanced Chronic Lymphocytic Leukemia (ACLL), and in the case of neurodegenerative diseases, such as Amyothrophic Lateral Sclerosis (ALS) [5].
Specifically in the latter case we have developed an Hough transform-based computational method for the segmentation of the spinal canal and the spinal cord in X-ray Computed Tomography (CT) images of ALS patients. Thus, information inferred from the anatomical images has been integrated with functional information from Positron Emission Tomography (PET) images in order to quantitatively evaluate the metabolic activity of the spinal marrow in control subjects and ALS patients. Results show that radiotracer uptake is significantly lower in spinal cord of controls as compared with patients.

References

[1] Beltrametti, M.C., Massone, A.M., and Piana, M. 2013 *Hough transform of special classes of curves*. SIAM Journal on Imaging Sciences 6(1), pp. 391–412.

[2] Duda, R.O., and Hart, P.E. 1972 *Use of the hough transformation to detect lines and curves in pictures*, Magazine Communications of the ACM, vol. 15(1), pp. 11–15.

[3] Hough, P.V.C. 1962 *Method and means for recognizing complex patterns*. U.S. Patent 3069654.

[4] Massone, A.M, Perasso, A., Campi, C., and Beltrametti, M.C. 2015 *Profile detection in medical and astronomical images by means of the Hough transform of special classes of curves*. Journal of Mathematical Imaging and Vision 51(2), pp. 296–310.

[5] Perasso, A., Campi, C., Massone, A.M., and Beltrametti, M.C., 2015 Spinal canal and spinal marrow segmentation by means of the Hough transform of special classes of curves. In *Image Analysis and Processing Ð ICIAP 2015*, V. Murino and E. Puppo, eds., 9279, Springer International Publishing.

Variational Image Enhancement Methods Enabling Strong Cost Reduction in OLED-based Point-of-care Immunofluorescent Diagnostic System

Patrizia Melpignano
OR-EL Organska elektronika d.o.o.
Volaričeva 6, 5222 Kobarid - Slovenia
office@or-el-doo.com

Stefano Bernardini
Università degli Studi di Bologna
Piazza di Porta S. Donato 5, 40126 Bologna - Italy
stefano.berarardini3@studio.unibo.it

The research in the field of point-of-care diagnostic for medical application has obtained an increased attention in the last years, world-wide. Among the main topics successfully addressed by this methodology there are: high detection sensitivity, portability, user friendly approach and reduced costs. All these are the key issues for a successful point-of-care diagnostic device. Currently, the new point of care diagnostic systems rely on different physical methods for the detection of the pathogens in a biological fluid; among the most sensitive and accurate methods, there is the detection of fluorescence of protein (inverse immunofluorescence) or DNA dye tagged probes. Based on this principle a multi-parametric biosensor has been developed and tested by OR-EL d.o.o., where an O-LED for the dye fluorescence excitation of a bio-probes matrix is used. This system currently use a high sensitivity scientific CCD camera to acquire the fluorescent image; this image sensor allows to obtain an excellent sensitivity but its size and cost make it rather unfit for a "low cost" point-of-care diagnostic application. In this talk, we present the results obtained with an alternative lower cost CMOS sensor by means of a three-phase post processing pipeline: a first restoration stage for noise reduction and resolution increase, a segmentation stage for the detection of samples, and a diagnosis stage for the calculation of the output concentrations. Each phase is formulated in a variational form and we test classical as well as state-of-the-art models for the purpose. Variational formulations are in general obtained by minimizing a functional which is the sum of a data fidelity term and a regularization term, based on a regularization operator chosen to yield a computed solution with some known desired features. A scalar parameter balances the influence of the fidelity and regularization terms on the computed solution in a suitable manner. We introduce metrics suitable for measuring the quality of the output and we present results obtained using three CMOS cameras, of significantly different costs, for the detection of the Dengue virus with a low-cost O-LED based detection system. Results demonstrate that our advanced processing pipeline enables cost reduction up to 99%, at an acceptable diagnostic accuracy, with respect to the reference CCD-based camera system.

3D restoration of prehistoric petroglyphs by photometric stereo

Giuseppe Rodriguez
Università di Cagliari
viale Merello 92, 09123 Cagliari, Italy
rodriguez@unica.it

Many regions of the Mediterranean area, such as Sardinia, are rich with prehistoric hypogeum tombs, dating back to the Neolithic up to the Bronze age, often characterized by engraved decorations. For archaeologists it is important to produce accurate reproductions of rock art engravings, but quite often the archeological sites are difficult to reach and their underground chambers are very narrow. In this situations, photometric stereo may provide an easy acquisition and low-cost technique to produce an accurate 3D reconstruction of the findings of interest. Data processing, from the mathematical point of view, consists of solving a least squares approximation problem, for determining local information about the observed surface, followed by the solution of a large scale partial differential equation, to determine a representation of its shape. The problem becomes difficult when the data acquisition setting is far from the ideal conditions, and when the position of the light sources is not exactly known. We will discuss some recent results on the application of this technique, with applications to the 3D restoration of engravings encountered in Sardinian Domus de Janas.

This work has been carried out in collaboration with R. Dessì, C, Mannu, G. Stocchino, G. Tanda and M. Vanzi, of the University of Cagliari.

References

[1] Dessì, R., Mannu, C., Rodriguez, G., Tanda, G., and Vanzi, M. 2015 *Recent improvements in photometric stereo for rock art 3D imaging.* Digital Applications in Archaeology and Cultural Heritage (DAACH), 2, 132–139.

The Role of Mathematical Modeling in Cultural Heritage: Research and Conservation

PROPOSERS

Giulio Magli
Politecnico di Milano
Pzza Leonardo da Vinci, 32 20133 - Milano Italy
Giulio.Magli@polimi.it

Roberto Natalini
Istituto per le Applicazioni del Calcolo, Consiglio Nazionale delle Ricerche
Via dei Taurini, 19, 00185 - Roma
roberto.natalini@cnr.it

SPEAKERS

Corrado Falcolini
Facoltà di Architettura, Università di Roma Tre
falco@mat.uniroma3.it

Barbara De Filippo
Istituto per le Applicazioni del Calcolo, Consiglio Nazionale delle Ricerche
roberto.natalini@cnr.it

Lucia Toniolo
Center for the Conservation and Valorisation of Cultural Heritage, Politecnico di Milano
lucia.toniolo@polimi.it

Antonio Bilotta
Univ. della Calabria
antonio.bilotta@unical.it

Giulio Magli
Dept. Mathematics, Politecnico di Milano
Giulio.Magli@polimi.it

The application of scientific techniques is today at the core of modern research on all aspects of cultural heritage: conservation, surveying, analysis and interpretation. Today a archaeological dig team includes experts in practically all fields of science, and mathematics is a key discipline in the analysis of the results. The same multi-disciplinary approach holds for research, conservation and fruition of existing archaeological sites and museums. The mini-symposium will touch a few of these issues related in particular to the mathematical modeling of degradation phenomena of materials as well as to modeling and virtual recreation of ancient monuments and landscapes and of their connection with the observation of the sky by their builders.

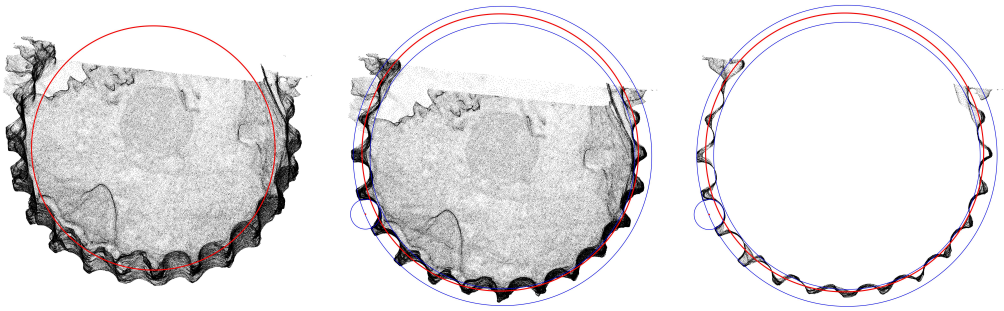
The Arch of Titus at the Circus Maximus in Rome: algorithms for virtual anastylosis.

Corrado Falcolini
Università degli Studi Roma Tre
via della Madonna dei Monti, 40 00184 - Roma Italy
falco@mat.uniroma3.it

A new accurate parametric model reconstruction of the Arch of Titus at the Circus Maximus in Rome is presented.
The model, based on surveyed fragments (old and new, some of them still in situ), historical knowledge and architectural order proportions, has been obtained also with the help of mathematical algorithms in several steps of the full process: the development of a database, containing more than 150 fragments of different size, using automatic feature extraction, contact surfaces detection and optimization of geometrical and parametrical description are only some of the developed applications.
The mathematical models are in a parametric form suited for improvements using features of all the known fragments and adaptable to successive findings: optimization is made possible by measures for an accurate quantitative analysis. The joint work (see [1]) with

M. Canciani and M. Saccone of the Department of Architecture and M. Buonfiglio and S. Pergola archeologists of the Sovrintendenza Capitolina ai Beni Culturali di Roma started with the collaboration of master students B. Mammí and G. Romito in 2012 and was followed by a first escavation of the area in 2013 (see also [2]). Many new pieces of the ancient arch were found during another operation in 2015; the final study was conducted also in collaboration with M. Pastor, A. Coletta and M.G. Granino.
Now the area has been finally open to the public with a documented visitor's itinerary along most of the arch fragments and a virtual anastylosis, based on our model, is presented using augmented reality on the site.

The database collects the point cloud of every fragment, by a survey done with a laser scanner and photogrammetry programs, together with a classification of several features suited for matching comparison. A general method has been proposed for a classification procedure adaptable for anastylosis in similar cases.
The algorithms discussed in this talk applied to a starting point cloud of a given fragment and deal with the best possible section curve on a plane orthogonal to the moulding extrusion path, an optimal fluting column model and contact probability of two possibly adjacent fragments.
The first example shows an automatic procedure (see [3]) for the extraction of a piecewise regular parametric curves of section directly from the point cloud: the plane of section can be detected analysing the normal components in the standard point cloud data, followed by a parametric planar curve fitting of properly selected points; special points on this parametric curve allow an automatic geometrical moulding construction which can be translated in feature elements of the database and used in matching procedures.
From the survey of a ruined column drum, the second algorithm example shows how it is possible to find an optimal fluted column model: comparing a cylindrical projection of the oriented point cloud with several section models, allows an optimal measure of column and flutings radii and then a possible drum reposition. The third example shows



the use of section curves for a precise fragment orientation and alignment: the required accuracy allowed a virtual segmentation of the surface of contact of two fragments of the inscription, leading to a final perfect matching and a better understanding of its probable size and shape.
All measures have been optimized up to a certain error using the processed data and have been verified and improved after any new fragment addition in the database.
Some of the original algorithms presented here have been also applied in different contexts: for instance several studies on the shape and tasselation of Borromini's San Carlino dome (see for example [4]), the recomposition and restoration of the fragmented statue of S. Andrea at Stiffe, L'Aquila (see [5]) or the bricks detection and analysis of masonry type of Villa dei Misteri in Pompei (see [6]).

References

[1] Canciani, M., Falcolini, C., Buonfiglio, M., Pergola, S., Saccone, M., Mammí, B., and Romito, G. 2013 *A method for virtual anastylosis: the case of the Arch of Titus at the Circus Maximus in Rome*. ISPRS Ann. Photogramm. Remote Sens. Spatial Inf. Sci., II-5/W1, 61–66.

[2] Canciani, M., Falcolini, C., Buonfiglio, M., Pergola, S., Saccone, M., Mammí, B., and Romito, G. 2014 *Virtual Anastylosis of the Arch of Titus at Circus Maximus in Rome*. International Journal of Heritage in the Digital Era, 3(2), 393–412.

[3] Canciani, M., Falcolini, C., Saccone, M. and Spadafora, G. 2013 *From Point Clouds to Architectural Models: algorithms for shape reconstruction*. ISPRS Ann. Photogramm. Remote Sens. Spatial Inf. Sci., XL-5/W1, 27–34.

[4] Falcolini, C., 2016 *Algorithms for Geometrical Models in Borromini's San Carlino alle Quattro Fontane*. Handbook of Research on Visual Computing and Emerging Geometrical Design Tools, 26, 642–665.

[5] Canciani, M., Capriotti, G., D'Alessandro, L., Falcolini, C. and Saccone, M. 2015 *The recomposition of fragmented objects: the case study of St. Andrea statue at Stiffe, L'Aquila*. XIII International Forum Le vie dei Mercanti, Heritage and Technology, Mind Knowledge Experience.

[6] Canciani, M., Falcolini, C., Saccone, M. and Spadafora, G. 2014 *From Point Cloud to Archaeology: the case study of Villa dei Misteri in Pompeii*. XII International Forum Le vie dei Mercanti, Best Practice in Heritage Conservation Management, From the World to Pompeii.

Material Damage: new mathematical models for the simulation of chemical processes.

Barbara De Filippo
Istituto per le Applicazioni del Calcolo Mauro Picone - CNR
Via dei Taurini 19 00185 Roma Italy
b.defilippo@iac.cnr.it

Roberto Natalini
Istituto per le Applicazioni del Calcolo Mauro Picone - CNR
Via dei Taurini 19 00185 Roma Italy
r.natalini@iac.cnr.it

In this work some recent mathematical models applied to material damage are reviewed. The complexity of damage processes related to Cultural Heritage materials creates the necessity of developing predictive tools in order to monitor and detect surface alterations even before they are visible by naked eyes. The proposed models, elaborated by a research group of the Institute of Applied Mathematics CNR of Italy, are based on partial differential equations and well capture the main features of chemical processes (copper corrosion and salt crystallization), which occur on different materials such as stone and copper.

Advanced nano-materials for the protection of stones in historic architecture

Lucia Toniolo
Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta", Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
lucia.toniolo@polimi.it

The development of nano-materials in the last two decades have found different application in the area of cultural heritage conservation [1]. The protection of stone materials in outdoor conditions is a rather important problem as it concerns historic and new high-quality buildings. The protection of stone materials addresses, generally, the main physical problem of the high hydrophilicity and wettability of these surfaces, as far as the presence of liquid and vapour water is able to favour all the deterioration phenomena like chemical corrosion, erosion and. Actually, the nanostructured protective materials can give water repellency together with other desirable effects like antifouling and anti-pollutants properties. The main and very interesting advantage of nanomaterials, compared with traditional treatments, is that they show high chemical-physical compatibility with substrates, higher reactivity, deeper penetration into the porosity when desired, higher aesthetic compatibility. The increasing interest in the design of innovative nanomaterials has been shown by the European Commission that launched different calls for proposal regarding the development of innovative materials for the conservation and restoration of Cultural Heritage both in 7thFP and Horizon 2020. For what concerns the improvement of stone protection, the most applied strategy has been the set-up of nanocomposites with the introduction of nanoparticles inside polymeric materialsin order to increase the hydrophobicity of stone surface and maintain their permeability and transparency. These treatments give rise to the so called superhydrophobic and self-cleaning surfaces, "Lotus leaf effect" [2]. The surface becomes water repellent and the residues of particulate matter or pollutants are removed and/or decomposed. In particular, the enhancement of water repellency can be achieved by increasing the surface roughness, without changing the substrate morphology, by the addition of different nanoparticles (SiO2, SnO2, Al2O3, TiO2). TiO2, ZnO and Ag nanoparticles have been proved to be also active to prevent the formation of surface biofilm, that is generally formed in northern exposition by the microorganisms colonization of stones. The anti-fouling activity of different nanoparticles and nano-composites[3, 4] is particularly interesting as far as the efficacy of preventive traditional treatments in this regard is rather modest. The wide differences in stone materials, in deterioration phenomena and in the actual nature of the real condition onsite, compel the researchers to perform large experimental set-up to test nanomaterials on different substrates both in the lab and onsite, to optimize the treatment and find the best practical conditions of application. The development of modeling of involved parameters (nanoparticle size, nature of solvents, layer thickness, depth of penetration, etc.) and of phenomena could, of course, greatly help in finding new solution for the protection of architectural surfaces.

References

[1] Baglioni P, Chelazzi D, Giorgi R *Nanotechnologies in the Conservation of Cultural Heritage. A compendium of materials and techniques.*, (2015) Springer, Netherlands.

[2] Parkin IP, Palgrave RG *Self-cleaning coatings.*, Journal of Materials Chemistry 2005, 15(17):1689-1695.

[3] Dalrymple OK, Stefanakos E, Trotz MA, Goswami DYA *Review of the mechanisms and modeling of photocatalytic disinfection.*, Applied Catalysis B: Environmental 2010, 98(1-2):27-38

[4] Bellissima F, Bonini M, Giorgi R, Baglioni P, Barresi G, Mastromei G, Perito B *Antibacterial activity of silver nanoparticles grafted on stone surface.*, Environ Sci Pollut Res 2014, 21(23):13278-13286

Analysis of historical masonry constructions through computational homogenization

Antonio Bilotta
Università della Calabria
via P. Bucci cubo 39C, 87036 - Rende (Cosenza) Italy
antonio.bilotta@unical.it

Andrea Causin
Università degli Studi di Sassari
via Garibaldi 35 Asilo Sella, 07041 - Alghero (Sassari) Italy
acausin@uniss.it

Margherita Solci
Università degli Studi di Sassari
via Garibaldi 35 Asilo Sella, 07041 - Alghero (Sassari) Italy
margherita@uniss.it

Emilio Turco
Università degli Studi di Sassari
via Garibaldi 35 Asilo Sella, 07041 - Alghero (Sassari) Italy
emilio.turco@gmail.com

The need for evaluating the structural safety of historic masonry constructions gave rise to many efforts aimed to device effective engineering methodologies in the recent years. See, for example, the review paper [1] and references therein. Among the methodologies based on FEM approaches it is possible, however, to distinguish the following main categories.

- *Micro modeling.* In micro modeling approaches, each constituent of the masonry, *i.e.* mortar and blocks, are described in the linear and nonlinear field by using damage or plasticity based laws, see for example [2]. In this way an accurate descripition of the problem is obtained but a huge computational effort is required. On the other hand, a remarkable advantage of the micro modeling is the use of constitutive parameters derived from experiments on units, joints and small masonry samples.

- *Macro modeling.* With macro modeling masonry is described as a fictitious continuum endowed with a proper set of parameters in order to characterize its linear an nonlinear response. See [3] for a plasticity based approach with softening behaviour and [4] for a specific damage model suitable for orthotropic brittle materials. The computational advantage of the macro modeling with respect to the micro modeling is clear, however the determination of the required continuum parameters involves not so simple tests on specimens of sufficiently large size.

It is then manifest how the formulation of numerical approaches for the analysis of masonry contructions is strongly conditioned by two fundamental requirements: the simplicity of

the experimental testing needed to evaluate the constitutive parameters – in this respect a great attention must to be devoted also to the preservation of the construction – and the sustainability of the computational costs. *Computational homogenization* [5], already tested in other contexts as composite materials, can be a viable approach having the advantage, as micro modeling, to require only the constitutive characterization of the single constituents, mortar and stone blocks. However, thanks to the two-scale micro-to-macro approach, it allows to limit the computational costs that can be considered intermediate between the costs required by a macro-analysis and those required a micro-analysis. With respect to other homogenization techniques does not require the preliminary definition of the macro response of the material which is, instead, defined *on the fly* by the computational strategy. The present work explored how computational homogenization can be used in the 3D finite element analysis of historic masonry constructions characterized by generic geometric configurations and whose masonry texture is given by a chaotic assemblage of irregular stones and mortar [6]. At the micro-level the FEM analysis is responsible to describe the nonlinear response of the rumble masonry. At the macro-level the FEM analysis of the assigned problem domain is responsible of the balance of the applied load conditions. In particular the two level of analysis dialogue as follows: the macro-level transfers to the micro-level the information regarding the displacement field, in particular its gradient, and the micro-level gives back the macro-stress and the tangent stiffness matrix of the RVE. In the work, in order to counteract the growing of computational costs, the use of high performance parallel numerical libraries and a mixed framework for obtaining more efficient finite elements [7] is proposed.

References

[1] P. Roca, M. Cervera, G. Gariup, L. Pelà, Structural Analysis of Masonry Historical Constructions. Classical and Advanced Approaches. *Archives of Computational Methods in Engineering*, 17 (2010) 299-325.

[2] S. Brasile, R. Casciaro, G. Formica, Multilevel approach for brick masonry walls - Part I: A numerical strategy for the nonlinear analysis. *Computer Methods in Applied Mechanics and Engineering*, 196 (2007) 4934–4951.

[3] P. B. Lourenco, R. de Borst, J. G. Rots, A plane stress softening plasticity model for orthotropic materials. *International Journal for Numerical Methods in Engineering*, 40 (1997) 4033–4057.

[4] L. Berto, A. Saetta, R. Scotta, R. Vitaliani, An orthotropic damage model for masonry structures. *International Journal for Numerical Methods in Engineering*, 55 (2002) 127–157.

[5] V. G. Kouznetsova, Computational homogenization for the multi-scale analysis of multi-phase materials (PhD thesis). Technische Universiteit Eindhoven (2002).

[6] F. Tedesco, A. Bilotta, E. Turco, Multiscale 3D mixed FEM analysis of historical masonry constructions *European Journal of Environmental and Civil Engineering*, (2016) DOI: 10.1080/19648189.2015.1134676.

[7] A. Bilotta, G. Garcea, L. Leonetti, A composite mixed finite element model for the elasto-plastic analysis of 3D structural problems. *Finite Element Analysis and Design*, 113 (2016) 43-53.

On going straight: mathematics and astronomy in the planning of ancient straight roads

Giulio Magli
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
giulio.magli@polimi.it

Many ancient cultures planned and constructed straight roads, sometimes taking an uttermost care in their "going straight". Astonishing examples can be found all around the world; for instance, among the Anasazi at Chaco Canyon, in many of the Maya *Sacbes*, at Angkor in the Khmer heartland, and of course, in the planning of the Roman roads. Among the latter, one stems out as a true masterpiece: it is *Regina Viarum*, the Via Appia. In many cases, geometrical and astronomical methods were applied to obtain a very high accuracy, especially along traits which are so long that the earth's curvature makes a direct view between the endpoints impossible. As it turns out, this "desire of going straight" was not always due to practical purposes but rather to symbolical, cosmological motivations. Sometimes, the very existence of the roads was connected mainly to such motivations. We discuss here some of the key examples in which the role of astronomy and geometry was essential in the planning.

References

[1] G. Magli, D. Sampietro, E. Realini, M. Reguzzoni *Uncovering a masterpiece of Roman architecture: the project of Via Appia between Collepardo and Terracina*, Journal of Cultural Heritage, Volume 15, 2014, 665-669

Stochastic Models for Fractional Processes

PROPOSERS

Gianni Pagnini
Ikerbasque & BCAM – Basque Center for Applied Mathematics
Alameda de Mazarredo, 14 48009 - Bilbao Basque Country–Spain
gpagnini@bcamath.org

SPEAKERS

Enrico Scalas (keynote)
Dept. of Mathematics, Univ. of Sussex UK
E.Scalas@sussex.ac.uk

Luisa Beghin
Dept. of Statistics, Univ. of Rome "La Sapienza"
luisa.beghin@uniroma1.it

Federico Polito
Dept. of Mathematics, University of Torino
federico.polito@unito.it

Francesco Di Tullio
University of Roma 3 & BCAM
francescoditullio91@gmail.com

Silvia Vitali
Dept. of Physics and Astronomy, Univ. of Bologna,
silvia.vitali4@unibo.it

Many processes in engineering and applied science exhibit behavior that cannot be modeled by classical methods [2, 4], this motivates and inspires research on new mathematical tools. One of this tools is Fractional Calculus. Fractional Calculus is a branch of analysis that studies nonlocal operators that can be understood as integration and derivation of non integer order and that reduce to classical operators in certain special cases. Successful applications of Fractional Calculus can be found in many disciplines as for example in chaotic Hamiltonian dynamics [5], biological systems [3], plasma physics [1]. These theoretical and modelling studies has led to new fundamental results. Part of these stochastic processes and models are for example the Lévy processes, the fractional Poisson procees, the continuos time random walk and the generalized gray Brownian motion. The aim of the minisymposium is to bring together researchers active in the development of stochastic processes and models related to phenomena governed by fractional differential equations. The talks are intended to be an exchange of recent results among researchers in the field and an up-to-date presentation for attendants of some important research lines and applications.

References

[1] del Castillo-Negrete, D. and Carreras, B. A. and Lynch, V. E. 2005 *Nondiffusive transport in plasma turbulence: A fractional diffusion approach*. Phys. Rev. Lett. 94, 065003.

[2] Metzler, R. and Klafter, J. 2004 *The restaurant at the end of the random walk: recent developments in fractional dynamics descriptions of anomalous dynamical processes*. J. Phys. A: Math. Theor. 37, R161–R208.

[3] Metzler, R. and Jeon, J.-H. and Cherstvy, A. G. and Barkai, E. 2014 *Anomalous diffusion models and their properties: non-stationarity, non-ergodicity, and ageing at the centenary of single particle tracking*. Phys. Chem. Chem. Phys. 16, 24128–24164.

[4] Tenreiro Machado, J. A. 2011 *And I say to myself: "What a fractional world!"*. Fract. Calc. Appl. Anal. 14, 635–654.

[5] Zaslavsky, G. M. 2002 *Chaos, fractional kinetics, and anomalous transport*. Phys. Rep. 371, 461–580.

Anomalous relaxation and continuous-time statistics

Enrico Scalas
University of Sussex
Department of Mathematics, Brighton BN1-9QH, UK
e.scalas@sussex.ac.uk

There is a deep connection between anomalous relaxation equations and continuous-time statistics of convolution type. As an illustrative example, consider the *maximum statistic*

$$S_n = \max(X_1, \ldots, X_n); \tag{1}$$

where X_is are positive random variables with the meaning of exceedances. Assume that sojourn times J_i are independent and identically positive random variables following a Mittag-Leffler distribution; in other words, the cumulative distribution function of J_1 is given by

$$F_{J_1}(t) = 1 - E_\alpha(-t^\alpha), \tag{2}$$

where

$$E_\alpha(z) = \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(n\alpha + 1)}$$

with $\alpha \in (0, 1)$. The corresponding continuous-time maximum statistics is

$$S(t) = \max(X_1, \ldots, X_{N_\alpha(t)}), \tag{3}$$

where $N_\alpha(t)$ is the fractional Poisson process of renewal type [1] defined as

$$N_\alpha(t) = \max\{n : \ J_1 + \ldots + J_n \leq t\}$$

Define $\mathcal{Q}(u, t)$ as

$$\mathcal{Q}(u, t) = F_{S(t)}(u) = \mathbb{P}(S(t) \leq u),$$

then the following anomalous relaxation equation holds true [2, 3]

$$\int_0^t \Phi_\alpha(t - t') \frac{\partial \mathcal{Q}(u, t')}{\partial t'} \, dt' = -(1 - F_{X_1}(u))\mathcal{Q}(u, t) \tag{4}$$

In (4), one has that $F_{X_1}(u) = \mathbb{P}(X_1 \leq u)$. Moreover, the kernel $\Phi_\alpha(t)$ is

$$\Phi_\alpha(t) = \frac{t^{-\alpha}}{\Gamma(1 - \alpha)}, \tag{5}$$

and the non-local relaxation equation can be written as

$$\frac{\partial^\alpha \mathcal{Q}(u, t)}{\partial t^\alpha} = -(1 - F_{X_1}(u))\mathcal{Q}(u, t), \tag{6}$$

where $\partial^\alpha / \partial t^\alpha$ is the Caputo derivative. The solution of (6) is

$$F_{S(t)}(u) = \mathcal{Q}(u, t) = E_\alpha(-(1 - F_{X_1}(u))t^\alpha), \tag{7}$$

where $E_\alpha(z)$ is the Mittag-Leffler function defined above. For $\alpha = 1$ (exponentially distributed sojourn times), and exponentially distributed X_1, one recovers the celebrated Gumbel distribution.
The structure outlined above can be generalised to other statistics of convolution type and this extention will be the subject of the presentation.

References

[1] F. Mainardi, R. Gorenflo and E.Scalas. A fractional generalization of the Poisson process. Vietnam Journal of Mathematics **32** SI 53–64 (2004).

[2] F. Mainardi, M. Raberto, R. Gorenflo and E. Scalas. Fractional calculus and continuous-time finance II: the waiting time distribution, Physica A **287**, 468–481 (2000).

[3] M.M. Meerschaert and B. Toaldo. Relaxation patterns and semi-Markov dynamics, `arXiv:1506.02951 [math.PR]` (2015).

Time-dependent fractional generators and related additive processes

Luisa Beghin
Sapienza Università di Roma
p.le A.Moro 5, 00185, Rome, Italy
luisa.beghin@uniroma1.it

Time-inhomogeneous, or additive, processes are obtained from Lévy processes by relaxing the condition of stationarity of increments. Due to the independence of their increments, additive processes are spatially (but not temporally) homogeneous Markov processes. By analogy with the case of Lévy processes, one can define an infinitesimal generator, which is, as a consequence, time-dependent. Additive versions of stable and Gamma processes have been studied, for example, in [5], [7], [6], [1], [8]. We consider here time-inhomogeneous generalizations of the well-known geometric stable processes, defined by means of time-dependent versions of fractional pseudo-differential operators of logarithmic type. The latter have been introduced and analyzed, in the time-homogeneous case, in [2], [3] and [4]. The corresponding local Lévy measures are expressed in terms of Mittag-Leffler functions with time-dependent parameters.

References

[1] Ayache A., Sharp estimates on the tail behavior of a multistable distribution, *Stat. Probab. Lett.*, 2013, 83, 3, 680–-688.

[2] Beghin L., Geometric stable processes and fractional differential equation related to them, *Electron. Commun. Probab.*, 2014, 19, 13, 1-14.

[3] Beghin L., Fractional gamma and gamma-subordinated processes, *Stoch. Anal. Appl.*, 2015, 33 (5), 903-926.

[4] Beghin L., Fractional diffusion-type equations with exponential and logarithmic differential operators, Arxiv 1601.01476v1, 2016, submitted.

[5] Cinlar E., On a generalization of Gamma processes, *Journ. Appl. Probab.*, 17, 2, 1980, 467-480.

[6] Falconer K., Liu L., Multistable processes and localisability, *Stochastic Models*, 2012, 28, 3, 503-526.

[7] Molchanova I., Ralchenko K., Multifractional Poisson process, multistable subordinator and related limit theorems, *Stat. Probab. Lett.*, 96, 2015, 95-101.

[8] Orsingher E., Ricciuti C., Toaldo B., Time-inhomogeneous jump processes and variable order operators, *Potential Analysis*, 2016, to appear.

Prabhakar Operators and Related Stochastic Processes

Federico Polito
Università degli Studi di Torino
via Carlo Alberto, 10 10123 - Torino Italy
federico.polito@unito.it

Prabhakar operators are convolution-type operator with a Prabhakar function (generalized Mittag-Leffler function) in the kernel. They generalize the classical Riemann–Liouville and Caputo fractional calculus operators and are connected to specific time-changed or subordinated stochastic processes. We discuss the results obtained in several articles and provide examples.

Fractional diffusion in complex media on the basis of Gaussian processes

Francesco Di Tullio
University of Roma Tre & BCAM - Basque Center for Applied Mathematics
Largo San Leonardo Murialdo, 1 00146 - Rome Italy
francescoditullio91@gmail.com

Gianni Pagnini
BCAM - Basque Center for Applied Mathematics & Ikerbasque
Alameda de Mazarredo, 14 E-48009 - Bilbao Basque Country - Spain
gpagnini@bcamath.org

Following the results presented in [1], we show the emergence of time-fractional and space-fractional diffusions from a Gaussian process when a distribution of random time-scales or random length-scales, respectively, characterises the medium where the diffusion takes place. Two different Gaussian models are considered in each case: in the case of time-fractional diffusion a standard Gaussian process with stretched random time and a Gaussian Continuous Time Random Walk (CTRW) model; in the case of space-fractional diffusion the fractional Brownian motion (fBm) and a Gaussian CTRW model. The stochastic process resulting from a Gaussian process with a random time is known as subordinated process. The stochastic process resulting from the fBm with a random length-scale is known as generalised gray Brownian motion (ggBm) [2, 3]. Each case leads to the desired solution with a specific distribution of the time-scales or space-scales accordingly. Hence, we show that for the same, and supposed experimentally observed, macroscopic fractional diffusion equation, e.g. the time-fractional or space-fractional diffusion equation, the characterisation of the medium at the mesoscale, which is given by the distribution of the time-scales and of the length-scales, respectively, allows for the determination of the underlying Gaussian microscopic process, i.e. a standard Gaussian process, the fBm or the Gaussian CTRW model.

References

[1] Pagnini, G. 2014 *Short note on the emergence of fractional kinetics*. Physica A 409, 29–34.

[2] Mura, M. and Pagnini, G. 2008 *Characterizations and simulations of a class of stochastic processes to model anomalous diffusion*. J. Phys. A: Math. Theor. 41, 285003.

[3] Pagnini, G. and Paradisi, P. 2016 *A stochastic solution with Gaussian stationary increments of the symmetric space-time fractional diffusion equation*. Fract. Cacl. Appl. Anal. 19, 408–440.

Fractional transport from the superposition of Ornstein–Uhlenbeck processes

Silvia Vitali
DIFA - Dipartimento di Fisica e Astronomia
Università degli Studi di Bologna
viale Carlo Berti Pichat, 6 40127 - Bologna Italy
silvia.vitali4@unibo.it

Paolo Paradisi
ISTI - Istituto di Scienza e Tecnologie dell'Informazione "Alessandro Faedo"
Area della Ricerca CNR di Pisa
Via G. Moruzzi, 1 56124 - Pisa Italy
paolo.paradisi@isti.cnr.it

Gastone Castellani
DIFA - Dipartimento di Fisica e Astronomia
Università degli Studi di Bologna
viale Carlo Berti Pichat, 6 40127 - Bologna Italy
gastone.castellani@unibo.it

Gianni Pagnini
BCAM - Basque Center for Applied Mathematics and Ikerbasque
Alameda de Mazarredo, 14 E-48009 - Bilbao Basque Country - Spain
gpagnini@bcamath.org

The Ornstein–Uhlenbeck (OU) process is driven by two physical parameters, the friction (equivalently, the relaxation or time correlation) and the noise intensity (equivalently the diffusivity). We discuss here the extension of the OU process by means of a random modulation of the same parameters. This random modulation can be interpreted as the effect of the statistical characteristics of the non-homogeneous/complex medium in which the diffusion occurs, e.g. the effect of random conditions in the experimental observations. In particular we show a parameter modulation that, when it is pluged into the Langevin equation, leads to fractional diffusion. After the results achieved on the basis of the generalized gray Brownian motion (ggBm) [1] and the Continuos Time Random Walk (CTRW) [2], the present approach is a further one based on the Langevin equation. These results support the physical idea that fractional diffusion in random/complex media can emerge from Gaussian processes for particle motion and random parameters due to the medium.

References

[1] Mura, M. and Pagnini, G. 2008 *Characterizations and simulations of a class of stochastic processes to model anomalous diffusion.* J. Phys. A: Math. Theor. 41, 285003.

[2] Pagnini, G. 2014 *Short note on the emergence of fractional kinetics*. Physica A 409, 29–34.

Fractional Processes: Analytical and Numerical Methods

PROPOSERS

Clemente Cesarano
International Telematic University Uninettuno, UTIU
Corso Vittorio Emanuele II, 39 00186 - Roma Italy
c.cesarano@uninettunouniversity.net

Gianni Pagnini
Ikerbasque & BCAM – Basque Center for Applied Mathematics
Alameda de Mazarredo, 14 48009 - Bilbao Basque Country–Spain
gpagnini@bcamath.org

Renato Spigler
"Roma Tre" University
Largo San Leonardo Murialdo, 1 00146 Rome - Italy
spigler@mat.uniroma3.it

SPEAKERS

Lidia Aceto
Deptartment of Mathematics, University of Pisa
lidia.aceto@unipi.it

Clemente Cesarano
Faculty of Engineering, UTIU
c.cesarano@uninettunouniversity.net

Renato Spigler
Dept. of Math. and Phys., "Roma Tre" University
spigler@mat.uniroma3.it

Gianni Pagnini
BCAM – Basque Center for Applied Mathematics and Ikerbasque
gpagnini@bcamath.org

Fractional Calculus is a branch of analysis concerning the study of nonlocal operators that can be interpreted as integrals and derivatives of non integer order [2]. It is wellknown that the first ideas on this topic go back to G.W. Leibniz (1695, 1697) and L. Euler (1730) and they have been developed up to nowadays [1]. Fractional Calculus is now widely applied in modelling in engineering and sciences [3] and the study of the corresponding fractional differential equations motivated the development of new analytical and numerical methods. These novel methods to solve fractional differential equations involve for example the theory and the applications of integral transforms and special functions, as well as new numerical strategies as for example those devised to improve the speed of convergence by means of an extrapolation method coupled with the *PageRank* algorithm. Some of these novel methods will be presented in this minisymposium.

References

[1] Baleanu, D. Diethelm, K. Scalas, E. and Trujillo, J. J. 2012 *Fractional Calculus: Models and Numerical Methods.* World Scientific.

[2] Oldham, K. B. and Spanier, J. 1974 *The Fractional Calculus.* Academic Press.

[3] Ortigueira, M. D. 2011 *Fractional Calculus for Scientists and Engineers.* Lecture Notes in Electrical Engineering, Springer.

Rational Approximation to the Fractional Laplacian Operator in Anomalous Diffusion Problems

Lidia Aceto
Università degli Studi di Pisa
via Filippo Buonarroti, 1/C 56127 - Pisa Italy
lidia.aceto@unipi.it

Paolo Novati
Università degli Studi di Trieste
via Valerio, 12/1 - 34127 Trieste Italy
novati@units.it

Fractional-order in space mathematical models, in which an integer-order differential operator is replaced by a corresponding fractional one, are becoming increasingly used since they provide an adequate description of many processes that exhibit anomalous diffusion. In this talk, in particular, we focus on the numerical solution of fractional in space reaction-diffusion equations on bounded domains under homogeneous Dirichlet boundary conditions. Using the matrix transform method, the fractional Laplacian operator is replaced by a matrix which, in general, is dense [1, 2]. The approach proposed is based on the approximation of this matrix by the product of two suitable banded matrices. This leads to a semi-linear initial value problem in which the matrices involved are sparse. The numerical experiments presented confirm the effectiveness of the proposed solution strategy.

References

[1] Ilić, M., Liu, F., Turner, I., Anh, V., 2005 *Numerical approximation of a fractional-in-space diffusion equation I.* Fract. Calc. Appl. Anal. 8, 323–341.

[2] Ilić, M., Liu, F., Turner, I., Anh, V., 2006 *Numerical approximation of a fractional-in-space diffusion equation (II)-with nonhomogeneous boundary conditions.* Fract. Calc. Appl. Anal. 9, 333–349.

Fractional operators and special polynomials

Clemente Cesarano
International Telematic University Uninettuno, UTIU
Corso Vittorio Emanuele II, 39 00186 - Roma Italy
c.cesarano@uninettunouniversity.net

The use of the translation operators techniques combined with some classes of orthogonal polynomials, as the generalized Hermite polynomials, is a powerful tool to describe the action of the exponential operators with fractional derivatives. Moreover, since the approach to fractional derivatives to deal with integral transform traces back to Riemann and Liouville and the combined use of ordinary transforms of Laplace or Fourier type can be exploited to define operators involving fractional power differential operators, it will discuss as the integral transforms providing the solution of some partial differential equations, as the heat equations, and in according with the Gauss transform, this method could be considered as a benchmark for the more general case employing some special family of generalized Hermite polynomials of the Kampé de Fériet type.

A perturbative approach to fractional differential equations

Renato Spigler
Roma Tre University
1, Largo S.L. Murialdo - 00146, Rome Italy
spigler@mat.uniroma3.it

Moreno Concezzi
Roma Tre University
1, Largo S.L. Murialdo - 00146, Rome Italy
concezzi@mat.uniroma3.it

Perturbation theory, both regular and singular, for fractional differential equations seems to be missing in the to date literature. On the other hand, such methods may be useful, either alternatively to or coupled with numerical methods, to construct approximate solutions. We present some sketchy theory along with few examples to illustrate the peculiarities of this field.

The effects of fractional diffusion on front propagation

Gianni Pagnini
BCAM – Basque Center for Applied Mathematics and Ikerbasque
Alameda de Mazarredo, 14 E-48009 - Bilbao Basque Country - Spain
gpagnini@bcamath.org

Andrea Mentrelli
University of Bologna, Department of Mathematics and $(AM)^2$
via Saragozza, 8 40123 - Bologna Italy
andrea.mentrelli@unibo.it

Andrea Trucchia
BCAM – Basque Center for Applied Mathematics
Alameda de Mazarredo, 14 E-48009 - Bilbao Basque Country - Spain
atrucchia@bcamath.org

Modelling the propagation of fronts and interfaces is a matter of paramount interest in many fields of science and engineering, such as those involving chemical reactions where the reacting interface separates two different compounds. Premixed turbulent combustion and wild-land fire propagation are two examples of such phenomena. Following [1, 2], a multi-dimensional model is presented to study the propagation of random fronts in media in which anomalous diffusion takes place. The anomalous diffusion is assumed here to be governed by a fractional diffusion equation. To track the position of the front at a certain time, the Level Set Method [3] is used. Since the propagation is assumed to occur in systems characterised by an underlying random motion the weighted mean of fronts calculated by means of the Level Set Method is performed. The weight function is the probability density function (PDF) which characterises the anomalous diffusion process. By using some case studies which emphasise the different dynamics with different kinetic (displacement variance and PDF) and geometrical (front curvature) configurations, several numerical experiments are presented and discussed.

References

[1] Mentrelli, A. and Pagnini, G. 2015 *Front propagation in anomalous diffusive media governed by time-fractional diffusion.* J. Comput. Phys. 293, 427–441.

[2] Mentrelli, A. and Pagnini, G. 2014 *Random front propagation in fractional diffusive systems.* Commun. Appl. Ind. Math. 6, e-504.

[3] Sethian, J. A. and Smereka, P. 2003 *Level set methods for fluid interfaces.* Annu. Rev. Fluid Mech. 35, 341–372.

Advanced Numerical Methods for Partial Differential Equations and Applications - Part I

PROPOSERS

Maurizio Falcone
Università La Sapienza di Roma
Piazzale Aldo Moro, 5 00185 - Roma, Italy
falcone@mat.uniroma1.it

Simona Perotto
MOX, Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano, Italy
simona.perotto@polimi.it

Gianluigi Rozza
SISSA, Area Matematica, MathLab
Via Bonomea, 265 34136 - Trieste, Italy
gianluigi.rozza@sissa.it

SPEAKERS

Matteo Aletti
Laboratoire Jacques-Louis Lions, UPMC, Paris
matteo.aletti@inria.fr

Simone Brugiapaglia
École Polytechnique Fédérale, Lausanne
simone.brugiapaglia@epfl.ch

Elisabetta Carlini
Università La Sapienza di Roma
carlini@mat.uniroma1.it

Nicola Ferro
MOX, Politecnico di Milano
nicola.ferro@polimi.it

Roberto Ferretti
Università Roma Tre
ferretti@mat.uniroma3.it

Matteo Giacomini
CMAP Ecole Polytechnique, Paris
matteo.giacomini@polytechnique.edu

This minisymposium proposes a state of the art of modern and advanced numerical methods for complex problems and systems governed by partial differential equations (PDEs) and a survey of possible applications. Topics include: optimization and control in several contexts, from shape optimization in fluids to Hamilton-Jacobi equations, mesh

adaptivity, accurate high-order methods, model order reduction. Concerning applications, the focus is mainly on advanced numerical methods for computational fluid dynamics, including iso-geometric analysis for viscous flows, model reduction for turbulent patterns, bifurcation and stability in fluids, multiphysics (fluid-structure interaction) problems, cardiovascular flows.

Reduced Steklov Operator for Multiphysics Systems

Matteo Aletti
Inria Paris & Sorbonne Universités UPMC Univ Paris 6
2 Rue Simone IFF, 75012 - Paris France
matteo.aletti@inria.fr

Damiano Lombardi
Inria Paris & Sorbonne Universités UPMC Univ Paris 6
2 Rue Simone IFF, 75012 - Paris France
damiano.lombardi@inria.fr

1 Introduction

The motivation of the present work is the study of the mechanics of the human eye. The eye is a complex system made of several fluid and solid compartments that interact with each other. In particular, we want to investigate the different phenomena that influence the intraocular pressure, which is an important quantity to be monitored in relation to several eye diseases such as, for instance, the Glaucoma. However, the computational costs of a 3D simulation of the eye can be prohibitive especially when taking into account several domains characterized by different physics. While the eye simulation will be the object of a future work, here we present a reduced technique to accelerate multiphysics simulations.

2 Mathematical framework

We consider a multiphysics system, see Fig.1, written on two domains, Ω_1 and Ω_2, that interact through an interface $\Gamma = \bar{\Omega}_1 \cup \bar{\Omega}_2$. The two domains do not have the same

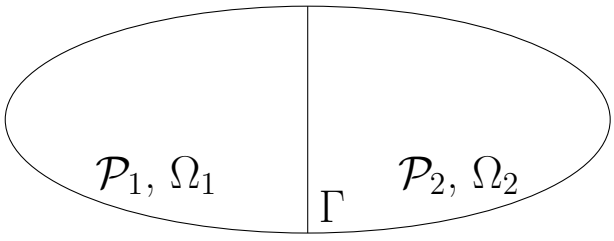


Figure 1: Geometrical setting with two different domains, Ω_1 and Ω_2, possibly characterized by different physics.

importance from the modeling viewpoint. In particular, we assume that the goal of the simulation is to have a precise description of the dynamics occuring into Ω_1, the *main problem* $\mathcal{P}_1$, while an accurate solution of the *secondary problem* $\mathcal{P}_2$ in Ω_2 is needed only because of the interaction occurring betweeen the two systems. The coupling is enforced via Domain Decomposition iterations (see, for instance, [1]). We solve time-dependent problems where several solutions of $\mathcal{P}_2$ are required: the goal of the proposed technique

is to solve $\mathcal{P}_2$ only a few times and, possibly, offline. We assume that the *secondary problem* is linear and that the boundary conditions on $\partial\Omega_2 \setminus \Gamma$, as well as the force terms, are constant in time. Different kinds of interface conditions are considered, such as Dirichlet to Neumann, Neumann to Dirichlet or Robin to Dirichlet. On the other hand, no assumptions are made on the *main problem*.
From the mathematical viewpoint, the most natural way to describe the dynamics of $\mathcal{P}_2$ is to use the Steklov operator. An example of such operator is the Dirichlet to Neumann map (D2N) that associates to a given Dirichlet datum $g \in H^{1/2}(\Gamma)$ the trace of the normal derivative of u, the solution of the problem $-\Delta u = 0$ on Ω_2. An extensive analysis on this subject can be found, for instance, in [2]. Even if the term Steklov operator is usually associated with the Laplace operator in the volume, we propose a method for a more general class of equations such as, for instance, the Stokes equations.

3 The reduced approach

The Steklov operator is non-local and therefore his finite-element matrix representation is a dense matrix of size $N_\Gamma \times N_\Gamma$, where N_Γ denotes the number of degrees of freedom on the interface. In order to build this matrix, N_Γ solutions of $\mathcal{P}_2$ are necessary. In several applications, such as the ones we are interested in, this matrix representation cannot be computed and stored.
In order to overcome this problem, we employ a very simple idea: we build a set of basis functions on Γ and we solve the *secondary problem* off-line for the first m ($m << N_\Gamma$) basis functions. The corresponding images of the Steklov operator will be used for the future online evaluations. The choice of the basis functions is important. The basis should be hierarchical, so that it is meaningful to take only the first m functions. The natural choice is to use the eigenfunctions of the Laplace-Beltrami operator defined on Γ because they are hierarchical and they also respect possible simmetries in the domain. They are computationally cheap to compute since it is enough to solve a sparse eigenproblem on the interface Γ.

Such an approximation of the Steklov operator can be interpreted as low-rank approximation where the Steklov eigenfunctions are approximated on the space spanned by the Laplace-Beltrami eigenfunctions.

We also remark that in simple geometries, where $\mathcal{P}_2$ can be analytically solved by separation of variables, the proposed approximation coincide with the low-rank one because the eigenfunctions of the Steklov operator and those of the Laplace-Beltrami operator are the same.
An interesting feature of this approach is that $\mathcal{P}_2$ is solved only in the off-line phase. This feature could be particularly useful when using different software for the different compartments. However, we also propose a way to perform an online update of the set of basis functions which requires the solution $\mathcal{P}_2$ during the online phase. We point out that the offline basis construction and the online update can be used alternatively or combined depending on the problem at hand and on the computational needs.

4 Results, conclusions and limitations

The reduced approach has been tested on some 3D numerical experiments. The results are consistent with the theoretical estimates on the convergence and on the computational costs. Three different systems have been tested so far: Stokes equations coupled with

a simplified fluid, Stokes equations coupled with the flow through a porous media and, finally, linear elasticity coupled with Stokes equations.
The results are encouraging in terms of speed up for the solution of the secondary problem. In particular, the online time dedicated to solve $\mathcal{P}_2$ is negligible compared to that used for problem $\mathcal{P}_1$. An interesting side effect is a slight reduction of the number of Domain Decomposition iterations, therefore reducing also the time dedicated to the solution of $\mathcal{P}_1$. As far as the online update is concerned, we obtained a good accuracy with a few online evaluations of the operator. We remark that the speed up of the entire simulations will depend mostly on the ratio between the sizes of the two problems. There are some limitations for using this approach: the method works on linear problems with force terms and boundary conditions that have to be constant in time. This for now limits the applicability of the method to quasi-static secondary problems.

Acknowledgements

This research was made possible by a Marie Curie grant from the European Commission in the framework of the REVAMMAD ITN (Initial Training Research network), Project number 316990.

References

[1] Quarteroni, A. and Valli, A. 1999 *Domain Decomposition methods for partial differential equations.* Oxford University Press.

[2] Khoromskij, B. and Wittum, G. 2012 *Numerical solution of elliptic differential equations by reduction to the interface*, vol. 36. Springer Science & Business Media.

Compressed sensing techniques for PDEs

Simone Brugiapaglia
École polytechnique fédérale de Lausanne
Route Cantonale, 1015 – Lausanne, Switzerland
simone.brugiapaglia@epfl.ch

Stefano Micheletti
MOX – Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 – Milano, Italy
stefano.micheletti@polimi.it

Fabio Nobile
École polytechnique fédérale de Lausanne
Route Cantonale, 1015 – Lausanne, Switzerland
fabio.nobile@epfl.ch

Simona Perotto
MOX – Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 – Milano, Italy
simona.perotto@polimi.it

We present the CORSING (COmpRessed SolvING) method for the sparse approximation of PDEs [1, 2, 3]. The goal is to reduce the computational cost associated with the Petrov-Galerkin discretization of a PDE by means of the *compressed sensing* technique, recently introduced in signal processing [4].
Establishing an analogy between the measurement of a signal and the Petrov-Galerkin discretization method, the bilinear form associated with the weak formulation of the PDE acts as a "virtual" sensing device. As a consequence, the application of compressed sensing allows for: (1) a dramatic dimensionality reduction, obtained through randomization of the test space associated with the Petrov-Galerkin discretization; (2) the recovery with high probability of the best s-term approximation to the unknown solution with respect to a suitable trial basis, via efficient sparse optimization tools – e.g., the *orthogonal matching pursuit* algorithm.
We assess the performance of CORSING applied to the advection-diffusion-reaction equation and to the Stokes problem, adopting *wavelets* as trial functions and a *trigonometric* basis as test basis (or vice versa). The robustness and the reliability of the method are shown by means of a MATLAB® numerical implementation and a theoretical analysis based on the concept of *local coherence* between bases is presented.

References

[1] S. Brugiapaglia. COmpRessed SolvING: Sparse Approximation of PDEs based on Compressed Sensing. Ph.D. thesis, MOX – Politecnico di Milano, 2016.

[2] S. Brugiapaglia, S. Micheletti, and S. Perotto. Compressed solving: A numerical approximation technique for elliptic PDEs based on Compressed Sensing. *Comput. Math. Appl.*, 70(6):1306–1335, 2015.

[3] S. Brugiapaglia, F. Nobile, S. Micheletti, and S. Perotto. A theoretical study of COmpRessed SolvING for advection-diffusion-reaction problems. Technical Report MOX-Report No. 42/2015, Politecnico di Milano, Dip. di Matematica, 2015.

[4] D.L. Donoho. Compressed sensing. *IEEE Trans. Inform. Theory*, 52:1289–1306, 2006.

A Semi-Lagrangian Scheme with Radial Basis Approximation for Surface Reconstruction

Elisabetta Carlini
Sapienza Università d Roma
Piazzale A. Moro 2, 00185 - Rome Italy
carlini@mat.uniroma1.it

Roberto Ferretti
Università Roma Tre
L.go S. Leonardo Murialdo, 1, 00146- Rome Italy
ferretti@mat.uniroma3.it

We propose a Semi-Lagrangian scheme accomplished with Radial Basis Function Interpolation for approximating a curvature-related level set model, which has been proposed by Zhao et al. in [7], to reconstruct unknown surfaces from sparse data sets. Semi-Lagrangian schemes for curvature-related equations have been first proposed in [3] and has gone through a number of improvements and applications, see in particular [1] for an in-depth convergence analysis. Successful technique for Surface Recostruction makes use of Radial Basis Functions, see for instance [5, 4, 2]. We take advantage of the two different approaches, in particular our scheme can solve the level set method on unstructured grids, with a consequent reduction of grid's dimension. Numerical tests show the behavior of our approach to reconstruct curves and surfaces.

References

[1] E. Carlini, M. Falcone and R. Ferretti, 2010 *Convergence of a large time-step scheme for Mean Curvature Motion.* Interf. Free Bound., **12**, 409–441.

[2] J.C. Carr, R.K. Beatson, J.B. Cherrie, T.J. Mitchell, W.R. Fright, B.C. McCallum and T.R. Evans, 2001 *Reconstruction and representation of 3d objects with radial basis functions.* Proceedings of ACM SIGGRAPH 2001, 67–76.

[3] M. Falcone and R. Ferretti, 2003 *Consistency of a large time-step scheme for mean curvature motion.* "Numerical Mathematics and Advanced Applications – ENUMATH 2001", 495–502, Springer.

[4] E. Franchini, S. Morigi, F. Sgallari, 2010 *Implicit shape reconstruction of unorganized points using PDE-based deformable 3D manifolds.* Numerical Mathematics: Theory, Methods and Applications, **3**,405–430.

[5] V.V. Savchenko, A.A. Pasko, O.G. Okunev and T.L. Kunii, 1995 *Function representation of solids reconstructed from scattered surface points and contours.* Computer Graphics Forum, **14**, 181–188.

[6] H. Wendland, 2005 *Scattered data approximation.* Cambridge University Press.

[7] H. Zhao, S. Osher, B. Merriman and M. Kang, 2000*Implicit and Non-parametric Shape Reconstruction from Unorganized Points Using Variational Level Set Method.* Computer Vision and Image Understanding, **80** 295–319.

Anisotropic Mesh Adaptation for Crack Propagation Induced by a Thermal Shock

Nicola Ferro
MOX- Dipartimento di Matematica, Politecnico di Milano
Piazza Leonardo da Vinci 32 I-20133, Milano, Italy
nicola.ferro@polimi.it

Simona Perotto
MOX- Dipartimento di Matematica, Politecnico di Milano
Piazza Leonardo da Vinci 32 I-20133, Milano, Italy
simona.perotto@polimi.it

Stefano Micheletti
MOX- Dipartimento di Matematica, Politecnico di Milano
Piazza Leonardo da Vinci 32 I-20133, Milano, Italy
stefano.micheletti@polimi.it

Corrado Maurini
Institut Jean Le Rond d'Alembert - Université Pierre et Marie Curie - Paris 6
4 Place Jussieu, 75252 Paris Cedex 05, France
corrado.maurini@upmc.fr

The variational model proposed in [1] includes thermal inelastic effects that describe the genesis and the propagation of cracks in brittle materials. In this context, the numerical modeling is usually performed via classical finite element schemes.

Regularized phase-field models of fracture exhibit two main length scales given by the domain size and the internal length characterizing the thickness of the smeared representation of the crack. The internal length is related to the limit stress in the material and it is typically very small with respect to the domain size.

In the context of uniform meshes, the coexistence of scales so different requires computational grids which are too fine, often making the computational effort prohibitive. Adaptive meshes can represent a remedy for containing the computational cost. Moreover, since fractures develop along definite directions, it can be computationally advantageous to exploit these intrinsic directionalities. Anisotropic adaptive meshes represent the ideal numerical tool with a view to a crack propagation modeling (see, e.g., [2]). Indeed, the employment of stretched elements can significantly reduce the cardinality of the mesh able to guarantee a desired accuracy on the solution.

Goal of this communication is to present a possible technique to generate an anisotropic adaptive mesh able to track crack evolution. For this purpose, we resort to an iterative procedure which combines the variational setting used to minimize the energy of the system at hand, with a metric-based mesh adaptive procedure driven by an anisotropic *a posteriori* estimator for the discretization error. The numerical verification performed on standard benchmarks in the literature confirms the good accuracy guaranteed by

anisotropic grids which yield also a significant computational saving. Particular care is devoted to the tuning of the parameters involved in the whole iterative procedure.

Finally, a first attempt of parameter identification is performed with a view to the simulation of more realistic configurations.

References

[1] Bourdin, B., Marigo, J.-J., Maurini, C., Sicsic, P., *Morphogenesis and Propagation of Complex Cracks Induced by Thermal Shocks*, Phys. Rev. Lett., 112 (1), 2014.

[2] Artina, M., Fornasier, M., Micheletti, S., Perotto, S., *Anisotropic mesh adaptation for crack detection in brittle materials*, SIAM J. Sci. Comput., 37 (4), 2015, B633-B659.

An Explicit, Semi-Lagrangian Advection–Diffusion Solver for the Navier–Stokes Equation

Roberto Ferretti
Università degli Studi Roma Tre
L.go S. Leonardo Murialdo, 1 00146 - Roma Italy
ferretti@mat.uniroma3.it

Luca Bonaventura
MOX - Politecnico di Milano
Via Bonardi, 9 20133 - Milano Italy
luca.bonaventura@polimi.it

Lorenzo Rocchi
Università degli Studi Roma Tre
L.go S. Leonardo Murialdo, 1 00146 - Roma Italy
lor.rocchi2@stud.uniroma3.it

Semi-Lagrangian (SL) schemes (see [1] for a recent, extensive review) stem from the so-called Courant–Isaacson–Rees scheme, and are known to have less restrictive stability conditions with respect to conventional Eulerian scheme. Despite being initially conceived for purely hyperbolic problems, in recent times they have been adapted and increasingly applied to parabolic equation, especially at high Reynolds numbers, or in case of degenerate operators. Their use leads in this case to an explicit advection–diffusion solver which remains uniformly stable for vanishing viscosity.
We will present a two-dimensional framework for integrating such a SL solver in a vorticity–streamfunction model for the Navier–Stokes Equation (see [3]), discussing advantages and drawbacks, and validating the code by some classical benchmarks. Preliminary tests [2] show that the scheme provides an efficient treatment of the advection–diffusion step, allows for relatively large Courant numbers and correctly captures the transition from laminar to turbulent regime.

References

[1] Falcone, M. and Ferretti, R. 2013 *Semi-Lagrangian Approximation Schemes for Linear and Hamilton–Jacobi Equations.* SIAM.

[2] Rocchi, L. 2016 *Solutori Semi-Lagrangiani per l'Approssimazione dell'Equazione di Navier–Stokes.* Tesi di Laurea, Università Roma Tre.

[3] Temam, R. 1984 *Navier–Stokes Equations: Theory and Numerical Analysis.* AMS.

An equilibrated fluxes approach to the Certified Descent Algorithm for shape optimization

Matteo Giacomini
CMAP Ecole Polytechnique
Route de Saclay 91128 - Palaiseau CEDEX France
matteo.giacomini@polytechnique.edu

Olivier Pantz
Université de Nice-Sophia Antipolis
Parc Valrose 06108 - Nice CEDEX 02 France
olivier.pantz@polytechnique.org

Karim Trabelsi
Institut Polytechnique des Sciences Avancées
15-21 Rue M. Grandcoing 94200 - Ivry-sur-Seine France
karim.trabelsi@ipsa.fr

In [3], we proposed a certification procedure to construct a genuine descent direction for a shape optimization problem approximated via the Finite Element Method. The resulting approach - named Certified Descent Algorithm (CDA) - accounts for the numerical error introduced by the discretization of the shape gradient to construct a guaranteed shape optimization strategy inspired by the Boundary Variation Algorithm [1]. The main features of the CDA are its ability to identify a genuine descent direction at each iteration of the procedure and the reliable stopping criterion for the overall optimization loop. In this talk, we discuss an improvement of the CDA which relies on the construction of a fully-computable goal-oriented estimator of the error in the shape gradient based solely on local quantities [2] via the equilibrated fluxes approach proposed by Mozolevski and Prudhomme in [4]. Some preliminary numerical tests for the inverse identification problem of Electrical Impedance Tomography are presented.

References

[1] Allaire, G. and Pantz, O. 2006 *Structural optimization with FreeFem++*. Struct. Multidisc. Optim. 32(3):173-181.

[2] Giacomini, M. 2016 *An equilibrated fluxes approach to the Certified Descent Algorithm for shape optimization using conforming Finite Element and Discontinuous Galerkin discretizations*. Submitted.

[3] Giacomini, M. and Pantz, O. and Trabelsi, K. 2016 *Certified Descent Algorithm for shape optimization driven by fully-computable a posteriori error estimators*. ESAIM: Control Optim. Calc. Var. *(to appear)*

[4] Mozolevski, I. and Prudhomme, S. 2015 *Goal-oriented error estimation based on equilibrated-flux reconstruction for finite element approximations of elliptic problems*. Comput. Methods Appl. Mech. Engrg. 288:127-145.

Advanced Numerical Methods for Partial Differential Equations and Applications - Part II

PROPOSERS

Maurizio Falcone
Università La Sapienza di Roma
Piazzale Aldo Moro, 5 00185 - Roma, Italy
falcone@mat.uniroma1.it

Simona Perotto
MOX, Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano, Italy
simona.perotto@polimi.it

Gianluigi Rozza
SISSA, Area Matematica, MathLab
Via Bonomea, 265 34136 - Trieste, Italy
gianluigi.rozza@sissa.it

SPEAKERS

Stefano Lorenzi
Politecnico di Milano
stefano.lorenzi@polimi.it

Simone Morganti
Università degli studi di Pavia
simone.morganti@unipv.it

Simona Perotto
MOX, Politecnico di Milano
simona.perotto@polimi.it

Annalisa Quaini
University of Houston
quaini@math.uh.edu

Gianluigi Rozza
SISSA MathLab
gianluigi.rozza@sissa.it

Filippo Salmoiraghi
SISSA MathLab
filippo.salmoiraghi@sissa.it

This minisymposium proposes a state of the art of modern and advanced numerical methods for complex problems and systems governed by partial differential equations (PDEs) and a survey of possible applications. Topics include: optimization and control in several contexts, from shape optimization in fluids to Hamilton-Jacobi equations, mesh

adaptivity, accurate high-order methods, model order reduction. Concerning applications, the focus is mainly on advanced numerical methods for computational fluid dynamics, including iso-geometric analysis for viscous flows, model reduction for turbulent patterns, bifurcation and stability in fluids, multiphysics (fluid-structure interaction) problems, cardiovascular flows.

A POD-Finite Volume-ROM Approach of Navier-Stokes and Turbulent RANS Equations for Industrial Applications

Stefano Lorenzi
Politecnico di Milano – Department of Energy
via la Masa 34 – 20156, Milano, Italy
stefano.lorenzi@polimi.it

Antonio Cammi
Politecnico di Milano - Department of Energy
via la Masa 34 – 20156, Milano, Italy
antonio.cammi@polimi.it

Lelio Luzzi
Politecnico di Milano – Department of Energy
via la Masa 34 – 20156, Milano, Italy
lelio.luzzi@polimi.it

Gianluigi Rozza
SISSA, International School for Advanced Studies, Mathematics Area, mathLab
via Bonomea 265 – 34136, Trieste, Italy
gianluigi.rozza@sissa.it

Numerical simulation of fluid flows requires important computational efforts but it is essential in engineering applications. Reduced Order Model (ROM) can be employed whenever fast simulations are required, or in general, whenever a trade-off between computational cost and solution accuracy is a preeminent issue as in process optimization and control [1], [2]. In this work [3], the efforts have been put to develop a ROM for Computational Fluid Dynamics (CFD) application based on Finite Volume approximation, starting from the results available in turbulent Reynold-Averaged Navier Stokes simulations in order to enlarge the application field of Proper Orthogonal Decomposition – Reduced Order Model (POD – ROM) technique to more industrial fields [4]. The approach is tested in the classic benchmark of the numerical simulation of the 2D lid-driven cavity. In particular, two simulations at $\mathrm{Re} = 10^3$ and $\mathrm{Re} = 10^5$ have been considered in order to assess both a laminar and turbulent case. Some quantities have been compared with the Full Order Model in order to assess the performance of the proposed ROM procedure i.e., the kinetic energy of the system and the reconstructed quantities of interest (velocity, pressure and turbulent viscosity). In addition, for the laminar case, the comparison between the ROM steady-state solution and the data available in literature has been presented. The results have turned out to be very satisfactory both for the accuracy and the computational times. As a major outcome, the approach turns out not to be affected by the energy blow up issue characterising the results obtained by classic turbulent POD-Galerkin methods. Finally, a parametrized reduced order model related to a nuclear

engineering problem is also presented to show a possible industrial application of the approach.

References

[1] Rozza, G., Huynh, D.B.P., Patera, A.T. 2008. *Reduced Basis Approximation and a Posteriori Error Estimation for Affinely Parametrized Elliptic Coercive Partial Differential Equations*. Arch. Comput. Methods Eng. 15, 229–275.

[2] Quarteroni, A., Rozza, G., Manzoni, A. 2011. *Certified reduced basis approximation for parametrized partial differential equations and applications*. J. Math. Ind. 1:3.

[3] Lorenzi, S., Cammi, A., Luzzi, L., Rozza, G., 2016. *POD-Galerkin Method for Finite Volume Approximation of Navier-Stokes and RANS equations*. Accepted for publication in Computer Methods in Applied Mechanics and Engineering.

[4] Wang, Z., Akhtar, I., Borggaard, J., Iliescu, T. 2012. *Proper orthogonal decomposition closure models for turbulent flows: a numerical comparison*. Comput. Methods. Appl. Mech. Eng. 237–240, 10–26.

Isogeometric analysis collocation: methodology and applications

Simone Morganti
Università degli Studi di Pavia
via Ferrata, 5 27100 - Pavia Italy
simone.morganti@unipv.it

Laura De Lorenzis
Technische Universitat Braunschweig
Pockelsstrasse 14, 38106 Braunschweig, Germany
l.delorenzis@tu-braunschweig.de

John Andrew Evans
University of Colorado Boulder
Boulder, CO 80309, Colorado USA
john.a.evans@colorado.edu

Thomas J.R. Hughes
University of Texas at Austin
201 E 24th St, Austin, TX 78712, Texas USA
tjr_hughes@hotmail.com

Alessandro Reali
Università degli Studi di Pavia
via Ferrata, 3 27100 - Pavia Italy
alessandro.reali@unipv.it

Isogeometric Analysis (IGA) is a recent analysis framework (cf. [1]) aiming at bridging Computational Mechanics and Computer Aided Design (CAD). It can be seen as an extension of standard isoparametric finite element methods, where the functions typically used by CAD systems (e.g., NURBS) are adopted to describe both geometry and field variables. In addition to clear advantages in terms of geometry representation capabilities, the use of such functions lead to superior results with respect to standard finite elements on a per degree-of-freedom basis, thanks to their high regularity properties [2]. In the framework of NURBS-based IGA, Isogeometric collocation has recently emerged as an innovative and promising numerical technique combining the high-order approximation properties and geometric flexibility of isogeometric analysis with the efficiency and simplicity of collocation schemes [3]. In this work, isogeometric collocation methods are applied for the first time to nearly incompressible plane strain elasticity. In particular, we focus on both $u-p$ and $\sigma-u$ mixed approaches, using an enriched displacement field with respect to the pressure/stress field and an equal-order equal-mesh method for displacement and pressure/stress. A very surprising result is that the equal-order methods are stable and attain "optimal" convergence rates. This is in stark contrast with the situation for equal-order Galerkin methods. Standard benchmarks from the literature,

including a 3D example, are studied showing that mixed collocation methods are able to overcome locking phenomena of the primal method occurring when approaching the incompressible limit.

References

[1] Cottrell, J.A., T.J.R. Hughes, and Y. Bazilevs 2009 *Isogeometric Analysis. Towards integration of CAD and FEA*. Wiley.

[2] Schillinger D., Evans, J.A., Reali, A., Scott, M.A., Hughes, T.J.R. 2013 *Isogeometric collocation: Cost comparison with Galerkin methods and extension to adaptive hierarchical NURBS discretizations.* Comp. Methods in Applied Mech. and Eng., 267, 170–232.

[3] Auricchio F., L. Beir‹o Da Veiga, T.J.R. Hughes, A. Reali, G. Sangalli 2012 *Isogeometric collocation for elastostatics and explicit dynamics.* Comp. Methods in Applied Mech. and Eng., 249, 2–14.

Hierarchical model reduction methods for incompressible fluids: basics, advances, applications

Simona Perotto
MOX, Dipartimento di Matematica, Politecnico di Milano
Piazza Leonardo da Vinci, 32. 20133 – Milano, Italy
simona.perotto@polimi.it

Hierarchical Model (HiMod) reduction methods provide surrogate models to describe phenomena with a dominant dynamics (e.g., blood flow in arteries, the hydrodynamics in river networks, the gasdynamics in an internal combustion engine), even though locally featuring relevant transverse components.
The driving idea of a HiMod reduction consists in a different discretization of the dominant and of the transverse dynamics, according to a separation of variables. In the original formulation [1], the mainstream is discretized via affine finite elements, and a modal approximation models the transverse dynamics. This approach leads to solve along the principal direction a "psicologically" one-dimensional model, whose coefficients automatically include the effect of the transverse dynamics. Additionally, the number of modes can be locally (and automatically) tuned along the mainstream, according to the meaningfulness of the transverse information [2]. Relatively few modes are expected to capture the transverse dynamics with an overall reduction of computational costs.
Our focus is on a haemodynamics setting. Thus, in this presentation, after introducing the basics for a HiMod reduction, we focus on the most recent advances of such an approach [3, 4]. In particular, we show a first application of the HiMod procedure to the blood flow modeling in a patient-specific stenotic coronary.
This is a joint work with Emory University in Atlanta, Universitá degli Studi di Pavia and University of Luxembourg. The support of clinical data by G. Guagliumi, Hospital Giovanni XXIII, Bergamo, is acknowledged.

References

[1] S. Perotto, A. Ern, and A. Veneziani. Hierarchical local model reduction for elliptic problems: a domain decomposition approach. *Multiscale Model. Simul.*, 8(4):1102–1127, 2010.

[2] S. Perotto and A. Veneziani. Coupled model and grid adaptivity in hierarchical reduction of elliptic problems. *J. Sci. Comput.*, 60(3):505–536, 2014.

[3] S. Perotto, A. Reali, P. Rusconi, and A. Veneziani. HIGAMod: a Hierarchical IsoGeometric Approach for MODel reduction in curved pipes. Accepted for the publication in *Comput. & Fluids*, 2016.

[4] D. Baroli, M.C. Cova, S. Perotto, L. Sala, A. Veneziani. Hi-POD reduction for the Navier-Stokes equations: towards hemodynamics applications. *In preparation* (2016).

A Large Eddy Simulation approach for incompressible flows at moderately large Reynolds numbers

Annalisa Quaini
Department of Mathematics
University of Houston, Houston (TX) USA
quaini@math.uh.edu

Luca Bertagna
Department of Scientific Computing
Florida State University, Tallahassee (FL) USA
lbertagna@fsu.edu

Alessandro Veneziani
Department of Mathematics and Computer Science
Emory University, Atlanta (GA) USA
avenez2@emory.edu

We consider a Leray model with a deconvolution-based indicator function for the simulation of incompressible fluid flow at moderately large Reynolds number (in the range of few thousand) with under-refined meshes. For the implementation of the model, we adopt a three-step algorithm called evolve-filter-relax (EFR) that requires the solution of a Navier-Stokes problem, the solution of a Stokes-like problem to filter the Navier-Stokes velocity field, and a final relaxation step [2]. We take advantage of a reformulation of the EFR algorithm as an operator splitting method to analyze the impact of the filter on the final solution vs a direct simulation of the Navier-Stokes equations. In addition, we provide some direction for tuning the parameters involved in the model based on physical and numerical arguments [1].
Our approach is validated against experimental data for fluid flow in an idealized medical device (consisting of a conical convergent, a narrow throat, and a sudden expansion, as recommended by the Food and Drug Administration). Numerical results are in good quantitative agreement with the measured axial components of the velocity and pressures for two different flow rates corresponding to turbulent regimes, even for meshes with a mesh size more than 40 times larger than the smallest turbulent scale. Through a large set of numerical experiments, we perform a preliminary sensitivity analysis of the computed solution to the parameters involved in the model.

References

[1] Bertagna, L. and Quaini, A. and Veneziani, A. 2015 *Deconvolution-based nonlinear filtering for incompressible flows at moderately large Reynolds numbers.* International Journal for Numerical Methods in Fluids, published online at http://dx.doi.org/10.1002/fld.4192.

[2] Bowers A.L. and Rebholz L.G. 2013 *Numerical study of a regularization model for incompressible flow with deconvolution-based adaptive nonlinear filtering.* Comput. Methods Appl. Mech. Eng., 258:1–12.

Reduced Order Methods: state of the art and perspectives with a focus on Computational Fluid Dynamics

Gianluigi Rozza
SISSA, International School for Advanced Studies, Mathematics Area, mathLab
via Bonomea, 265 34136 - Trieste Italy
gianluigi.rozza@sissa.it

In this talk we deal with the state of the art of Reduced Order Methods (ROM) for parametric Partial Differential Equations (PDEs) [3] and we provide some perspectives in their current trends and developments, with a special interest in Computational Fluid Dynamics (CFD) parametric problems. Systems modelled by PDEs are depending by several complex parameters in need of being reduced, even before the computational phase in a pre-processing step. Efficient parametrizations (random inputs, geometry, physics) are very important to be able to properly address an offline-online decoupling of the computational procedures and to allow competitive computational performances. Current ROM developments include: a better use of high fidelity methods, also spectral element method, enhancing the quality of the reduced model too [5]; more efficient sampling techniques to reduce the number of the basis functions, retained as snapshots, and the dimension of online systems; the improvements of the certification of accuracy based on residual based error bounds and stability factors; for nonlinear system also investigations on bifurcations of parametric solutions is crucial and it may be obtained thanks to a reduced eigenvalue analysis [6]. All the previous aspects are very important in CFD problems in order to be able to study complex industrial and biomedical flow problems in real time, and to couple viscous flows -velocity, pressure, and also thermal field - with a structural field [1] or a porous medium [4]. This last task requires also an efficient reduced parametric treatment of interfaces [2].

References

[1] F. Ballarin, G. Rozza, POD-–Galerkin monolithic reduced order models for parametrized fluid-structure interaction problems, *Int. Journal Num. Meth. Fluids*, in press, 2016.

[2] D. Forti, G. Rozza, Efficient geometrical parametrisation techniques of interfaces for reduced-order modelling: application to fluid–-structure interaction coupling problems, *Int. Journal Comp. Fluid Dyn.* Volume 28, Issue 3-4, pp 158-169, 2014.

[3] J. S. Hesthaven, G. Rozza, B. Stamm, Certified Reduced Basis Methods for Parametrized Partial Differential Equations, Springer Briefs in Mathematics, 2015.

[4] I. Martini, G. Rozza, B. Haasdonk, Reduced basis approximation and a-posteriori error estimation for the coupled Stokes-Darcy system, *Advances in Computational Mathematics*, Volume 41, Issue 5, pp 1131-1157, 2015.

[5] G. Pitton, G. Rozza, A reduced basis method for bifurcation problems in incompressible fluid dynamics, *submitted*, 2015. SISSA preprint 55/2015/MATE.

[6] G. Pitton, A. Quaini, G. Rozza, Computational reduction strategies for bifurcations and stability analysis in fluid-dynamics: applications to Coanda effect, *submitted*, 2016.

Reduced Order Methods for Automotive and Nautical applications

Filippo Salmoiraghi
SISSA (International School for Advanced Studies)
via Bonomea, 265 34136 - Trieste Italy
filippo.salmoiraghi@sissa.it

Gianluigi Rozza
SISSA (International School for Advanced Studies)
via Bonomea, 265 34136 - Trieste Italy
gianluigi.rozza@sissa.it

Angela Scardigli
OPTIMAD Engineering Srl
Via Giacinto Collegno, 18 10143 - Torino Italy
angela.scardigli@optimad.it

Haysam Telib
OPTIMAD Engineering Srl
Via Giacinto Collegno, 18 10143 - Torino Italy
haysam.telib@optimad.it

We present a new computational pipeline for the Model Order Reduction, from the geometrical parametrization to the construction of the reduced basis, for complex design problems in engineering. The proposed approach relies on Free Form Deformation (FFD) for the geometrical parametrization, an improved "leave one out" strategy for the selection of the parameters value, and Proper Orthogonal Decomposition (POD) with interpolation of the POD coefficients for the online real-time evaluation. Since most of the time design engineers are interested in the outputs of a problem instead of the global solution, both the parameters selection and reduced basis construction are performed directly on the output of interest. After a general presentation of the methodology and computational pipeline and some results in motor yachts field, we show the application to the solution of steady RANS equations around the *drivAer* [1] model with parametric bumper shape. The outputs of interest, for example, are the pressure and wall stress fields on the car, which are fundamental for the computation of drag and lift coefficients. The results show a significant computational speed-up of order of millions with an error of about 4%. Alongside we briefly present two new python toolkit libraries developed at SISSA mathLab suited and designed for the model order reduction, namely *PyGeM* [2] and *EZyRB* [3].

References

[1] drivAer website: http://www.drivaer.com

[2] PyGeM website: https://github.com/mathLab/PyGeM

[3] EZyRB website: https://github.com/mathLab/EZyRB

[4] Salmoiraghi, F., Ballarin, F., Heltai, L., Rozza, G.: Isogeometric analysis based reduced order modelling for incompressible viscous flows in parametrized shapes: applications to underwater shape design (2015).

Approximation Methods for Data, Images and Operators

PROPOSERS

Mariantonia Cotronei
DIIES, Università Mediterranea di Reggio Calabria
Via Graziella, loc. Feo di Vito, 89122 Reggio Calabria, Italy
mariantonia.cotronei@unirc.it

Francesca Pitolli
Dipartimento SBAI, Università di Roma "La Sapienza"
Via Antonio Scarpa 16, 00161 Roma, Italy
francesca.pitolli@sbai.uniroma1.it

Luigia Puccio
Dipartimento MIFT, Università di Messina
Viale Ferdinando Stagno d'Alcontres 31, 98166 Messina, Italy
gina@unime.it

SPEAKERS

Cristina Campi
Dipartimento SBAI, Università di Roma "La Sapienza"
cristina.campi@sbai.uniroma1.it

Francesca Pitolli
Dip. SBAI, Università di Roma "La Sapienza"
francesca.pitolli@sbai.uniroma1.it

Lucia Romani
Dipartimento di Matematica e Applicazioni, Università di Milano-Bicocca
lucia.romani@unimib.it

Milvia Rossini
Dipartimento di Matematica e Applicazioni, Università di Milano-Bicocca
milvia.rossini@unimib.it

Gianluca Vinti
Dipartimento di Matematica ed Informatica, Università di Perugia
gianluca.vinti@unipg.it

Mariantonia Cotronei
Dipartimento di Informatica, Matematica, Elettronica e Trasporti, Università Mediterranea di Reggio Calabra
mariantonia.cotronei@unirc.it

The proposed mini-symposium is related to the activities of the SIMAI Activity Group "SIMAI-SIMA", whose aim is to promote and coordinate research activities on mathematical models and numerical methods for experimental data analysis, CAGD,

automation, animation, signal processing, image processing, scientific visualization, virtual reality.
The mini-symposium is intended to bring together researchers from different fields working on signal/image processing and approximation methods with the aim of presenting and sharing novel techniques, research results, and experience. A special emphasis will be put on the applications to real-world problems, from computer aided design to biomedical applications.
In particular, the confirmed speakers participating in the mini-symposium will present research advances both in the construction of suitable methods for data analysis (sampling, radial basis functions, multiple multiresolution analysis) and in the application to real-world problems (PET data analysis, tomographic image processing, anomalous viscoelestic damping).

Some finite bounds for testing the Hough regularity of special classes of algebraic curves

Cristina Campi
Dipartimento SBAI, Università degli Studi di Roma "La Sapienza"
via A. Scarpa 14, 00160 - Roma Italy
cristina.campi@sbai.uniroma1.it

Maria Laura Torrente
CNR - IMATI
Via dei Marini, 6, 16149 - Genova Italy
laura.torrente@ge.imati.cnr.it

Hough transform [2] is a well-known pattern recognition technique for the recognition of straight lines and ellipses in images. Recently, it has been extended to families of algebraic curves [1] and applied to real data [3], like X-ray computed tomography (CT) images.

Let us consider a family of non-constant irreducible real polynomials:

$$F(X,Y;\lambda)=\sum_{i,j=0}^{d} g_{ij}(\lambda)X^iY^j,\ \ 0\le i+j\le d, \tag{1}$$

in the variables X, Y, where $\lambda=\lambda_1,\cdots,\lambda_t$ are real parameters and the coefficients $g_{ij}(\lambda)$ are evaluations of real polynomials $g_{ij}(\Lambda)$ in the indeterminates $\Lambda=(\Lambda_1,\ldots,\Lambda_t)$. Let $\mathcal{F}$ be the corresponding family of zero loci $\mathcal{C}_\lambda$ of $F(X,Y;\lambda)$, and assume that each $\mathcal{C}_\lambda$ is an irreducible real curve in the affine plane $\mathbb{A}^2_{(X,Y)}(\mathbb{R})$, i.e., $\mathcal{C}_\lambda$ is an irreducible curve over the complex field with infinitely many real points in $\mathbb{A}^2_{(X,Y)}(\mathbb{R})$. If $P=(x_P,y_P)$ is a point of $\mathbb{A}^2_{(X,Y)}(\mathbb{R})$, then the Hough transform of P (with respect to the family $\mathcal{F}$) is defined by the equation $\Gamma_P(\Lambda): F(x_P,y_P;\Lambda)=0$, where

$$F(x_P,y_P;\Lambda)=\sum_{i,j=0}^{d} g_{ij}(\Lambda)x_P^iy_P^j,\ \ 0\le i+j\le d, \tag{2}$$

is a real polynomial in the indeterminates $\Lambda=(\Lambda_1,\ldots,\Lambda_t)$. The following general facts hold true [1].

(a) *The Hough transforms $\Gamma_P(\mathcal{F})$, when P varies on $\mathcal{C}_\lambda$, all pass through the point λ.*

(b) *Assume that the Hough transforms $\Gamma_P(\mathcal{F})$, when P varies on $\mathcal{C}_\lambda$, have a point in common other than λ, say λ'. Thus the two curves $\mathcal{C}_\lambda$, $\mathcal{C}_{\lambda'}$ coincide.*

(c) (Regularity property) *The following conditions are equivalent*:

  (i) *For all curves $\mathcal{C}_\lambda$, $\mathcal{C}_{\lambda'}$ in $\mathcal{F}$, the equality $\mathcal{C}_\lambda=\mathcal{C}_{\lambda'}$, implies $\lambda=\lambda'$.*

  (ii) *For each curve $\mathcal{C}_\lambda$ in $\mathcal{F}$, one has $\bigcap_{P\in\mathcal{C}_\lambda}\Gamma_P(\mathcal{F})=\lambda$.*

The Hough regularity property, involving the infinite intersection of the Hough transforms of all the points on the curve, although theoretical solid, can be neither satisfied nor tested in the case of real, discretized data. Further, the computation of the intersection of the Hough transforms is the key step of the procedure for detecting an algebraic curve (the recognition algorithm), since it provides the parameters of the curve $\mathcal{C}_\lambda$ best approximating the given dataset. Therefore, it is natural to ask whether $\cap_{p\in\mathcal{C}_\lambda}\Gamma_p(\mathcal{F})$ can be rewritten as a finite intersection and how many Hough transforms are needed to define it. Under mild assumptions, we provide two bounds for the finite intersection. We compute these bounds for several algebraic curves and we test the robustness of these values when the recognition algorithm is employed with noisy data.

References

[1] Beltrametti, M. C., Massone, A. M., Piana, M. 2013 *Hough transform of special classes of curves*. SIAM Journal on Imaging Sciences 6, 391–412.

[2] Hough, P. V. C. 1962 *Method and means for recognizing complex patterns*. US Pat. 3069654.

[3] Massone, A. M., Perasso, A., Campi C., Beltrametti, M. C. 2015 *Profile detection in medical and astronomical images by means of the Hough transform of special classes of curves*. Journal of Mathematical Imaging and Vision 51, 296–310.

A wavelet Galerkin-collocation method for a fractional diffusion equation

Francesca Pitolli
Dip. SBAI, Università di Roma "La Sapienza"
Via A. Scarpa, 16 00191 - Roma Italia
francesca.pitolli@sbai.uniroma1.it

Laura Pezza
Dip. SBAI, Università di Roma "La Sapienza"
Via A. Scarpa, 16 00191 - Roma Italia
laura.pezza@sbai.uniroma1.it

Fractional differential equations have gained a great interest in the last decades. In fact, the memory (in time) or local (in space) effect due to fractional derivatives allows to model real world phenomena in a realistic way [3]. In particular, fractional differential equations are extensively used to model anomalous diffusion in several materials, like viscous fluids, porous media or biological tissues.
In this talk we present a wavelet method to solve the *fractional-in-time differential diffusion problem*

$$\begin{cases} D_t^\gamma u(t,x) - \dfrac{\partial^2}{\partial x^2} u(t,x) = f(t,x)\,, & t \in [0,T]\,, \quad x \in [0,1]\,, \\ u(0,x) = 0\,, & x \in [0,1]\,, \\ u(t,0) = u(t,1) = 0\,, & t \in [0,T]\,, \end{cases} \tag{1}$$

where $D_t^\gamma u$, $0 < \gamma < 1$, denotes the *partial fractional derivative* with respect to the time t (for definition and properties of the fractional derivative see, for instance, [3]).
The proposed method combines a wavelet collocation method in time and a wavelet Galerkin method in space that use the fractional wavelets associated to the fractional refinable functions introduced in [1] as approximating functions. The main advantage is in that both fractional and integer order derivatives of the fractional wavelets can be evaluated by a closed form that involves just the fractional difference operator [2]. We will show the effectiveness and efficiency of the method by some numerical tests.

References

[1] Pezza, L. 2007 *Fractional GP refinable functions*, Rend. Mat. VII. 27, 73–87.

[2] Pezza, L. and Pitolli, F. 2016 *A multiscale collocation method for fractional differential problems*, submitted.

[3] Podlubny, I. 1999 *Fractional differential equations*, Mathematics in Science and Engineering, vol. 198, Academic Press.

Corner cutting net subdivision schemes

Lucia Romani
Università degli Studi di Milano-Bicocca
via R. Cozzi, 55 20125 - Milano Italy
lucia.romani@unimib.it

Costanza Conti
Università degli Studi di Firenze
viale Morgagni, 40/44 50134 - Firenze Italy
costanza.conti@unifi.it

Nira Dyn
University of Tel-Aviv
10 Mezada St. Hod Hasharon 45294 - Tel-Aviv Israel
niradyn@math.tau.ac.il

Net subdivision schemes are iterative algorithms to generate bivariate continuous functions by recursively refining nets of continuous univariate functions defined on grids of intersecting lines in the plane. In this talk we extend to nets of functions the corner cutting algorithm for sequences of points, initially investigated by Carl de Boor [1] to define univariate subdivision schemes for curve generation. Assuming that the corner cutting weights satisfy analogous conditions as those considered in the point setting by Gregory and Qu [2], we prove that corner cutting algorithms for nets of functions converge to bivariate continuous functions whenever the initial net consists of univariate continuous functions that are Lipschitz continuous on grid intervals.

References

[1] de Boor, C. 1987 *Cutting corners always works.* Comput. Aided Geom. Design 4(1-2), 125–131.

[2] Gregory, J.A., Qu, R. 1996 *Nonuniform corner cutting.* Comput. Aided Geom. Design 13, 763–772.

On directional scaling matrices in dimension $d = 2$

Milvia Rossini
Università di Milano Bicocca
via via Cozzi, 55 20125 - Milano Italy
milvia.rossini@unimib.it

Scaling matrices are the key ingredient in subdivision schemes and multiresolution analysis, because they fix the way to refine the given data and to manipulate them. It is known that the absolute value of the scaling matrix determinant gives the number of disjoint cosets which is strictly connected with the number of filters needed to analyze a signal and then to computational complexity. Among the classical scaling matrices, we find the family of shearlet matrices that have many interesting property that make them attractive when dealing with anisotropic problems. Their drawback is their relatively large determinant. The aim of this paper is to discuss systems of scaling matrices with the same good properties of shearlet matrices but with lower determinant.

Approximation methods by sampling type operators with applications to Digital Image Processing

Gianluca Vinti
Università degli Studi di Perugia
Dipartimento di Matematica e Informatica
Via Vanvitelli, 1 06123 - Perugia Italy
gianluca.vinti@unipg.it

The aim of this talk is to show that the theory of multivariate sampling type operators play a fundamental role in signal analysis and it has important applications to Digital Image Processing, see [1, 2, 3, 5, 6, 7]. In particular, we will discuss some recent applications to CT images for the study of vascular diseases. We will show how the implementation of the theory developed by the sampling type operators (see e.g., [5]), along with other Digital Image Processing algorithms, is useful for the diagnosis of abdominal aortic aneurysms (see e.g., [4]). Also recent applications to Energy Engineering will be examined.

References

[1] Bardaro, C., Butzer, P.L., Stens, R.L. and Vinti, G. 2007 *Kantorovich-type generalized sampling series in the setting of Orlicz spaces*. Sampl. Theory Signal Image Process. 6 (1), 29-52.

[2] Bardaro, C., Musielak, J. and Vinti, G. 2003 *Nonlinear Integral Operators and Applications.* New York, Berlin: De Gruyter Series in Nonlin. Anal. and Appl. 9.

[3] Costarelli, D. Minotti, A.M. and Vinti, G. 2016 *Approximation of discontinuous signals by sampling Kantorovich series,* submitted.

[4] Costarelli, D., Seracini, M. and Vinti, G. 2015 *Digital image processing algorithms for diagnosis in arterial diseases.* Proceedings in Applied Mathematics and Mechanics.

[5] Costarelli, D. and Vinti, G. 2013 *Approximation by nonlinear multivariate sampling Kantorovich type operators and applications to image processing*. Num. Funct. Anal. Opt. 34 (6), 819-844.

[6] Costarelli, D and Vinti, G. 2014 *Rate of approximation for multivariate sampling Kantorovich operators on some functions spaces*. Journal of Integral Equations and Applications, 26 (4), 455-481.

[7] Vinti, G. and Zampogni, L. 2014 *Approximation results for a general class of Kantorovich type operators*. Advanced Nonlinear Studies 14, 991-1012.

Hermite subdivision and multiwavelets with polynomial-exponential cancellation properties

Mariantonia Cotronei
Università degli Studi Mediterranea di Reggio Calabria
via Graziella - loc. Feo di Vito, 89122 - Reggio Calabria, Italy
mariantonia.cotronei@unirc.it

This talk deals with Hermite subdivision schemes, which are efficient iterative procedures for refining vector data, with the particular understanding that these vectors represent function values and consecutive derivatives up to a certain order.
In particular, we focus on the preservation capabilities of such schemes when acting on elements in the space spanned by exponential and polynomials, and we show that this property is related to the possibility of factorizing the (level-dependent) subdivision operator in terms of the so-called annihilator operator.
Such a factorization is the key for the construction of a class of Hermite-type multiwavelet filters possessing polynomial/exponential vanishing moments, which turn out to be useful in a wide range of applications.

Derivative-Free and Simulation-Based Optimization

PROPOSERS

Margherita Porcelli
Università degli Studi di Firenze, Department of Industrial Engineering
viale Morgagni, 40/44 50134 - Firenze Italy
margherita.porcelli@unifi.it

Francesco Rinaldi
Università di Padova, Department of Mathematics
via Trieste, 63 35121 Padova - Italy
rinaldi@math.unipd.it

SPEAKERS

Guido Cocchi
DINFO, Università degli Studi di Firenze
guido.cocchi@unifi.it

Andrea Manno
DEIB, Politecnico di Milano
andrea.manno@polimi.it

Silvia Poles
Noesis Solutions
silvia.poles@noesissolutions.com

Margherita Porcelli
DIEF, Università degli Studi di Firenze
margherita.porcelli@unifi.it

Elisa Riccietti
DiMaI, Università degli Studi di Firenze
elisa.riccietti@unifi.it

Francesco Rinaldi
Dept. of Mathematics, Università di Padova
rinaldi@math.unipd.it

The efficient solution of optimization problems arising in real applications increasingly calls for the development of efficient and easy-to-use implementations of derivative-free algorithms. In applicative contexts such as engineering design, medical image registration and design of algorithms (amongst many others), optimization problems are often defined by functions computed by costly simulation. A single simulation performed to evaluate the costly function may, for instance, require the solution of large systems of partial differential equations or even a costly measurement campaign, and hence, may take from a few minutes to many hours or days depending on the particular application. Functions have therefore to be treated as expensive black-boxes and due to the high computational cost involved, it is important to use optimization algorithms that produce reasonably

good solutions within a limited number of function evaluations. Moreover, optimization variables can be of different nature: continuous (e.g. geometrical parameters), integer (e.g. on/off element of a structure) or more generally categorical variables, which are discrete variables which identify an element of an unordered set (e.g. colors, shapes, or materials). The aim of this symposium is to present new advances in the solution of simulation based optimization problems via derivative-free optimization. The analyzed problems range from single and multi-objective nonlinear problems to multilevel problems of the min-max type and cover the cases of continuous and mixed-integer variables. Special attention will be devoted to the application of the proposed algorithms to real-life problems and to the discussion of implementation issues. Specifically, applications comprise:

- optimization of the start-up phase of a concentrated solar power plant;
- parametric design of centrifugal pumps;
- design of electrical wiring interconnection system for aircrafts;
- automatic parameter estimation of codes.

An implicit filtering-based algorithm for derivative free multiobjective optimization

Guido Cocchi
Università degli Studi di Firenze
Dip. Ingegneria dell'Informazione, Via di S.Marta, 3 50139 - Firenze Italy
guido.cocchi@unifi.it

Giampaolo Liuzzi
Consiglio Nazionale delle Ricerche (IASI - CNR)
Istituto di Analisi dei Sistemi ed Informatica "A. Ruberti",Via dei Taurini 19 00185 - Roma - Italy giampaolo.liuzzi@iasi.cnr.it

Alessandra Papini
Università degli Studi di Firenze
Dip. Ingegneria Industriale, Viale Morgagni, 40/44 50134 - Firenze Italy
alessandra.papini@unifi.it

Marco Sciandrone
Università degli Studi di Firenze
Dip. Ingegneria dell'Informazione, Via di S.Marta, 3 50139 - Firenze Italy
marco.sciandrone@unifi.it

In this work we consider multiobjective optimization problems with bound constraints. We assume that the objective functions are continuously differentiable and that their gradients are not available. We present an algorithm combining direct search and implicit filtering approaches. At each iteration, a multiobjective variant of the classical coordinate search is performed. The implicit filtering phase starts whenever the coordinate search is unsuccessful, i.e. the coordinate search cannot produce a new nondominated point. The computed objective function values are employed to approximate the gradients of the objective functions, and a linear programming problem is solved to define a possible multiobjective descent direction. Then, a line search is performed along the computed direction. Global convergence results are stated, computational experiments are performed and the obtained results are presented and discussed.

Numerical optimization of the start-up phase of a Concentrated Solar Power plant

Andrea Manno
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
andrea.manno@polimi.it

Edoardo Amaldi
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
edoardo.amaldi@polimi.it

Francesco Casella
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
francesco.casella@polimi.it

Emanuele Martelli
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
emanuele.martelli@polimi.it

Stefano Trabucchi
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
stefano.trabucchi@polimi.it

Operational flexibility is the key feature for next generation power plants. The main flexibility requirements are (1) high efficiency part-load operation, (2) quick load changes (ramp-up, ramp-down) and (3) reduced start-up and shut-down times. This work focuses on the optimization of the start-up phase of an advanced Concentrated Solar Power (CSP) plant using molten salts as heat carrier with a high temperature storage system. While the optimization of the part-load steady-state operation is relatively straightforward, the optimization of the quick load changes and start-up/shut-down operations is a very challenging optimal control problem because of the complex dynamic models which are involved. Given the differential algebraic equations which describe the dynamic behavior of the power plant relating state variables with boundary conditions and control variables, it is necessary to determine the values of the control variables at each time instant $u(t)$ which lead to the minimum of a performance function (e.g., start-up time). Constraints are also included so as to avoid excessive mechanical stresses of the plant components and solidification of the molten salts. Due to the large number of state variables of the system and relatively small number of control variables, a single-shooting approach has been considered: like in black-box optimization, the optimization algorithm tunes the values of the control variables, and, for each solution sampled, the dynamic model is solved with

an ad hoc solver (e.g., DYMOLA, OpenModelica). Since computational time required by each dynamic simulation is very high, computing first and second order information is prohibitive. Hence we adopted a model-based derivative-free optimization algorithm tailored for costly function evaluations.

References

[1] Holmstrom, K., Quttineh, N. H., Edvall, M. M. 2008. *An adaptive radial basis algorithm (ARBF) for expensive black-box mixed-integer constrained global optimization* Optimization and Engineering, 9(4), 311-339.

[2] Björkman, M., Holmstrom, K. 2000. *Global optimization of costly nonconvex functions using radial basis functions* . Optimization and Engineering, 1(4), 373-397.

Electrical Wiring Interconnection System (EWIS) for aircraft

Silvia Poles
Noesis Solutions NV
Gaston Geenslaan 11, 3001 - Leuven Belgium
silvia.poles@noesissolutions.com

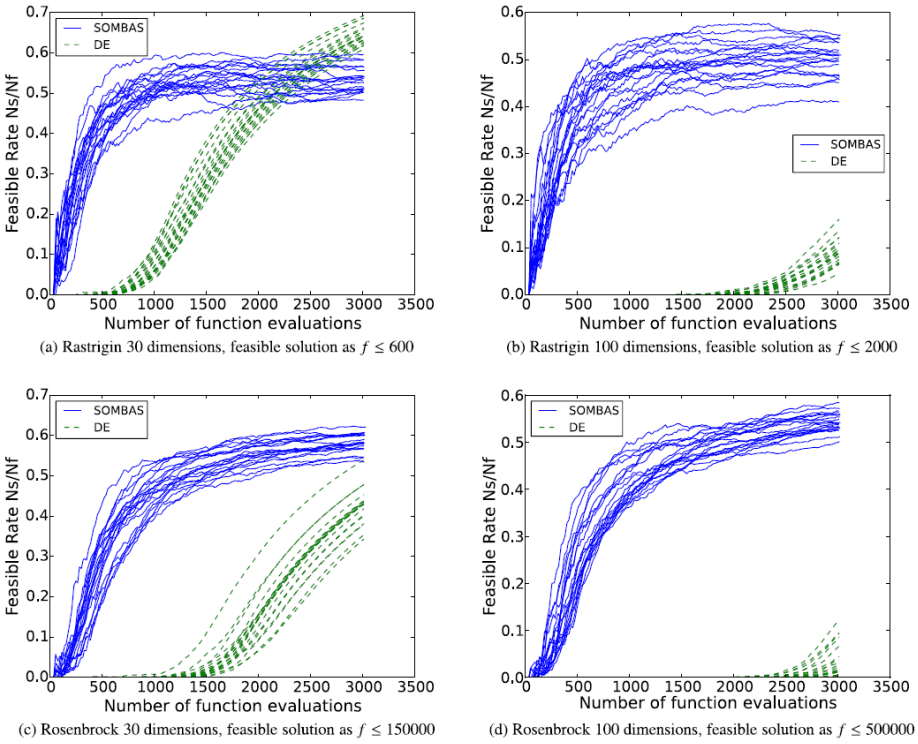
Keiichi Ito
Noesis Solutions NV
Gaston Geenslaan 11, 3001 - Leuven Belgium
keiichi.ito@noesissolutions.com

Roberto d'Ippolito
Noesis Solutions NV
Gaston Geenslaan 11, 3001 - Leuven Belgium
roberto.dippolito@noesissolutions.com

Solving the problem of complexity might be one of the major goals of the 21st century: in the engineering field this is translated into high number of parameters to take into consideration as development projects are getting bigger and often too complex to be grasped entirely by one single person. In particular, complexity in aircraft is increasing significantly, incorporating more electric systems than before. For example, subsystems that were used to be pneumatic or hydraulic are now replaced by electric components. On top of that, charging capabilities and in-flight entertainment programs are now provided to all passengers. The wire harnesses that are used to connect all those systems together must now also convey more signals and power. From the point of view of design engineers, this requirement results in a high number of parameters to consider during the development process.

Electrical systems are used for flight control, sensors, engine control, flight management, communication, in-flight entertainment and for many other purposes in the aircraft. The connection of all these systems is done by what is called the *Electrical Wiring Interconnection System* (EWIS). This is the entire collection of electrical wiring, connectors, bus bars, shielding, sleeves, pressure seals, brackets, etc. For manufacturing and production purposes, the entire wiring system is produced in modular components. Each component is called *wire harnesses* and is the component to which all the wires are bundled. At the final assembly all these modular components are integrated into one full EWIS by connecting everything back together.

In this paper, a 48 harnesses optimization problem is use which is well representing the complexity described above. The strategies use to solve this complex problem are demonstrated. In this optimization problem we want to find the configuration with the minimum weight, the total weight is given by the cables sizing. Moreover, all functional constraints for electrical design (around $10,000$ constraints for the maximum voltage drop) and for thermal design (around $40,000$ for the maximum overheating) should be fulfilled. Given the large amount of design variables ($10,000$ variables representing the



(a) Rastrigin 30 dimensions, feasible solution as $f \leq 600$

(b) Rastrigin 100 dimensions, feasible solution as $f \leq 2000$

(c) Rosenbrock 30 dimensions, feasible solution as $f \leq 150000$

(d) Rosenbrock 100 dimensions, feasible solution as $f \leq 500000$

Figure 1: Evolution of feasible rate Ns/Nf of SOMBAS and Differential Evolution on two different test functions with increasing dimensions [1].

size of the cables) and the number of constraints that describe the design space of real gauge sizing problems, the challenge of optimizing such system has to be considered as a high-dimensional, non-linear and a mixed integer problem with a mixing of discrete and continuous input variables. In this kind of problems, not only optimizing, but even finding a feasible solution can be consider a difficult task.
The use of machine learning techniques, an optimization approach based on the use of Self-Organizing Maps (SOM) [2] (Self-Organizing Map Based Adaptive Sampling - SOMBAS [1], see fig 1) and other techniques have contributed to an adaptive optimization strategy to solve this EWIS problem. The fundamental idea of the SOMBAS approach is an algorithm that learns to select new samples in the region of interest, using the density learning mechanism that is used for SOM. The complete strategy put in place has successfully demonstrated the optimization of high dimensional systems and particularly the ability in finding feasible solutions for highly constrained problems.

References

[1] Keiichi Ito, Ivo Couckuyt, Roberto d'Ippolito, and Tom Dhaene. 2016. Design space exploration using Self-Organizing Map based adaptive sampling. In *Appl. Soft Comput.* vol. 43, pp. 337–346.

[2] J. Kangas, T. Kohonen, Developments and applications of the self-organizingmap and related algorithms, Math. Comput. Simul. 41 (1996) 312.

Optimization of algorithms with BFO, a trainable derivative-free Brute Force Optimizer for nonlinear problems with mixed variables

Margherita Porcelli
Università degli Studi di Firenze
viale Morgagni, 40 50134 - Firenze Italy
margherita.porcelli@unifi.it

Philippe L. Toint
University of Namur
61, rue de Bruxelles, B5000 - Namur, Belgium
phtoint@unamur.be

Parameter tuning has widespread applications because it addresses a widespread problem: improving performance [2]. This performance is typically measured on the basis of a number of specific metrics reported by the algorithm after it has been run on valid input data. As an example, a measure of performance may consist in the number of iterations required by a nonlinear equation solver, in the number of objective gradient evaluations in an optimization solver, in the performed CPU time, etc. Algorithmic performance, be it in optimization or any other field, depend more or less critically on a number of parameters. The estimation of these parameters is extremely important to ensure the best algorithmic performance for the broadest class of problems and to provide reliable default settings to non-expert users. Some parameters may be real numbers, such as an initial trust-region radius, but they may also be discrete, such as the maximal number of iterations, or even categorical, such as a Boolean indicating whether exact or inexact Hessian is used. Moreover, these parameters may be required to remain between two, possibly infinite bounds, or may be constrained in a more complex way.
In the framework of the works [1, 2], in this talk we provide formalizations of the parameter-tuning problem that enables us to treat it as a blackbox optimization problem and provide a solution strategy based on derivative-free direct-search methods.
More generally, we present a new Matlab optimizer called BFO (Brute-Force Optimizer) for bound-constrained nonlinear (and possibly nonsmooth) problems. We assume that the evaluation of the objective function is time-consuming, and that no derivative is available. Moreover, no convexity assumption is made. Remarkable features of BFO are its ability to handle a mix of continuous and discrete variables, a versatile interface as well as a novel self-training option. Its performance compares favourably with that of NOMAD, a state-of-the art package. It is also applicable to multilevel equilibrium- or constrained-type problems. Its easy-to-use interface provides a number of user-oriented features, such as checkpointing and restart, variable scaling and early termination tools. The BFO code is freely available at https://sites.google.com/site/bfocode/.

References

[1] Audet, C., Orban, D. 2006 *Finding optimal algorithmic parameters using derivative-free optimization.* SIAM J. Opt. 17(3), 642–664.

[2] Audet, C., Dang, K. C., and Orban, D. 2014 *Optimization of algorithms with OPAL.* Math. Prog. Comp. 6(3), 233–254.

Support Vector Machine applied to the parametric design of centrifugal pumps

Elisa Riccietti
Università degli Studi di Firenze, DIMAI
Viale Morgagni 67/a, 50134 - Firenze Italy
elisa.riccietti@unifi.it

Andrea Arnone
Università degli Studi di Firenze, DIEF
Via di Santa Marta 4, 50134 - Firenze Italy
andrea.arnone@unifi.it

Juri Bellucci
Università degli Studi di Firenze, DIEF
Via di Santa Marta 4, 50134 - Firenze Italy

Matteo Checcucci
Università degli Studi di Firenze, DIEF
Via di Santa Marta 4, 50134 - Firenze Italy

Michele Marconcini
Università degli Studi di Firenze, DIEF
Via di Santa Marta 4, 50134 - Firenze Italy

The aerodynamic and mechanical redesign of a turbomachinery component lead to analyze the performance of components with complex three-dimensional geometry, described by tens of geometrical parameters. Thus, the design space investigated becomes really vast and a lot of points are necessary to adequately sample it. Each point in the design space corresponds to a geometry that should be processed through Computational Fluid Dynamics (CFD) computations. However, the competitiveness of the business requires the design process to be as short as possible, so computationally expensive CFD calculations are usually coupled with regression meta-models, such as Artificial Neutral Networks (ANN).
A regression model for each objective function defining the machine performance is built, to be applied to new geometries. However, it is impossible to take a priori into account of all the manufacturing or geometrical constraints. As an outcome, the most part of the analyzed geometries will result not feasible from a manufacturing point of view, or will reach a poor computational convergence. As a consequence a very high number of CFD computations has to be performed to generate a reasonably large training set of feasible geometries for the meta-model, as the most part of them turns out to be useless. Moreover, once the regression model is obtained it cannot be used to predict function values for randomly selected points of the design space, as it would yield meaningless values if an unfeasible geometry is found.
We present a strategy to overcome the aforementioned problem. The standard approach

based on CFD and ANN as a regression meta-model is coupled with Support Vector Machine (SVM). SVM is used as a classification meta-model with the aim of detecting the unfeasible parameters combinations among the samples randomly chosen in the design space. This has two benefits: it avoids useless CFD calculations during the ANN training phase, and it helps limiting the prediction of the objective functions values through the regression model to the feasible samples.
The results of this strategy applied to the parametric design of centrifugal pumps for a wide range of specific speeds are reported.

A new derivative-free method for integer programming problems

Francesco Rinaldi
Dipartimento di Matematica - Università degli Studi di Padova
via Trieste, 64 35121 - Padova Italy
rinaldi@math.unipd.it

Giampaolo Liuzzi
Istituto di Analisi dei Sistemi ed Informatica "Antonio Ruberti" (IASI) - Consiglio Nazionale delle Ricerche (CNR)
Via dei Taurini 19, 00185 - Roma Italy
liuzzi@iasi.cnr.it

Stefano Lucidi
Dipartimento di Ingegneria Informatica, Automatica e Gestionale - Università degli Studi di Roma, La Sapienza
via Ariosto, 25 00100 - Roma Italy
lucidi@dis.uniroma1.it

In this work, we consider integer programming problems with both bound constraints on the variables and general nonlinear constraints, where objective and constraint function values can only be obtained by querying a black box. We define a new derivative-free method that combines the use of suitably generated sets of search directions with a specific penalty approach. Furthermore, we report the results of some preliminary numerical experiments on both bound constrained and nonlinearly constrained problems.

Learning, games, and optimization - Part I

PROPOSERS

Roberto Lucchetti
Politecnico di Milano
Pzza Leonardo da Vinci, 32 20133 - Milano Italy
roberto.lucchetti@polimi.it

Lorenzo Rosasco
Università di Genova
Via Dodecaneso, 35 16146 Genova Italy
lrosasco@mit.edu

Silvia Villa
Istituto Italiano di Tecnologia
Via Morego, 30 16100 Genova Italy
silvia.villa@iit.it

SPEAKERS

Nicolò Cesa-Bianchi (keynote)
Dip. di Informatica, Univ. di Milano
nicolo.cesa-bianchi@unimi.it

Nicola Basilico
Università degli Studi di Milano
nicola.basilico@unimi.it

Tomáš Kroupa
Dip. di Matematica, Univ. di Milano
Tomas.Kroupa@unimi.it

Fabio Nobile
École Polytechnique Fédérale de Lausanne
fabio.nobile@epfl.ch

Marcello Pelillo
Dip. di Scienze Ambientali, Informatica e Statistica, Univ. Ca' Foscari Venezia
marcello.pelillo@gmail.com

Analytics, decision, and artificial intelligent systems have been recently revolutionized by data driven technologies fuelled with data of unprecedented size and complexity. The challenge of defining flexible models and data exploration strategies is paralleled by the need of efficiently processing big data-sets in possibly very high dimensions. The techniques to be employed arise from a combination of ideas and tools from a variety of diverse fields. Three main such fields are machine learning, game theory, and optimization. The goal of this mini-symposium is to gather experts from these fields to discuss mathematical challenges and potentially unveil novel connections.

Relevance to SIMAI The challenges of modern data driven technologies ask for new sound solutions and novel synthesis of ideas from different fields of mathematics. The mini-symposium on the "Mathematics of learning from data" we organized in the 2014 meeting had a good impact in terms of interest and audience. We believe that the proposed mini-symposium offers a unique opportunity to foster new collaborations and engage the italian applied mathematics community with the many opportunities of a new emerging field.

Online Learning via Sketching

Nicolò Cesa-Bianchi
Università degli Studi di Milano
via Comelico 39, 2015 Milano
nicolo.cesa-bianchi@unimi.it

Haipeng Luo
Princeton University
Princeton, NJ USA

Alekh Agarwal
Microsoft Research
New York, NY USA

John Langford
Microsoft Research
New York, NY USA

Online learning methods quickly reduce the prediction risk on large, high-dimensional datasets. First order methods are particularly attractive as they typically enjoy computational complexity linear in the input size. However, the convergence of these methods crucially depends on the geometry of the data: running the same algorithm on a rotated set of examples can return vastly inferior results. Second order algorithms, such as Online Newton Step [1], have the attractive property of being invariant to linear transformations of the data, but typically require space and update time quadratic in the number of dimensions. In this work we describe a new online second order algorithm with provably good regret guarantees for ill-conditioned data. The algorithm is an enhanced version of Online Newton Step and uses sketching techniques to achieve a linear running time in the dimension (or even linear in the number of non-zero entries in case of sparse data). While the idea of data sketching is widely studied [2], as far as we know this work is the first one to apply it to the adversarial online learning setting providing rigorous regret guarantees. See the full paper [3] for more details.

References

[1] Elad Hazan, Amit Agarwal, and Satyen Kale. Logarithmic regret algorithms for online convex optimization. *Machine Learning*, 69(2-3):169–192, 2007.

[2] David P Woodruff. Sketching as a tool for numerical linear algebra. *Foundations and Trends in Machine Learning*, 10(1-2):1–157, 2014. ISSN 1551-305X. doi:10.1561/0400000060.

[3] Haipeng Luo, Alekh Agarwal, Nicolò Cesa-Bianchi, and John Langford. Efficient Second Order Online Learning via Sketching. *arXiv preprint arXiv:1602.02202*, 2016.

Algorithms for Computing a Leader–Follower Equilibrium with Multiple Followers

Nicola Basilico
Università degli Studi di Milano
via Festa del Perdono, 7 20122 - Milano Italy
nicola.basilico@unimi.it

Stefano Coniglio
University of Southampton
Highfield Southampton SO17 1BJ - Southampton UK
s.coniglio@soton.ac.uk

Nicola Gatti
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
nicola.gatti@polimi.it

The introduction of the so–called leader–follower (or Stackelberg) equilibrium [5] has deeply influenced the Artificial Intelligence community, playing a central role in the study and deployment of many real–world applications (specifically in the security domain, e.g. [4]). The computational problem of finding a leader–follower equilibrium is well assessed for settings with one follower [1]. Differently, for games with multiple followers the results available in the literature are only sporadic. In this setting, a wide spectrum of scenarios arises and different properties can be observed, according to the nature of the game played by the followers. In this paper, we focus on the case where the followers play a Nash equilibrium [2] once the leader's strategy is given. Under such terms, the problem of finding a leader–follower equilibrium is well–defined only when, given the strategy of the leader, the followers play the Nash equilibrium that is optimal for the leader (a.k.a. optimistic case). Instead, when the followers play a Nash equilibrium that is not optimal for the leader (including the case in which they play the worst Nash equilibrium for the leader, a.k.a. pessimistic case), the leader–follower equilibrium may not exist and only somehow approximated equilibria should be considered.

First, we show that the problem of finding a leader–follower equilibrium with 2 or more followers is not in Poly–APX unless P=NP even with Polymatrix games, and this result holds both in the optimistic and pessimistic cases. More precisely, we show that it is unlikely that there is a polynomial–time algorithm approximating the utility of the leader at the leader–follower equilibrium within a polynomial ratio in the number of actions of the players.

Next, we propose a number of algorithms based on non–linear mathematical programming to find an equilibrium, exploring both the general case in which players act in mixed strategies and the restricted case in which some player (i.e., either the leader or the followers) acts in pure strategies. Furthermore, we study both the optimistic case and the pessimistic case (here accepting a strategy profile in which the loss of the leader is

bounded by ϵ). We conclude by providing a thorough experimental evaluation based on a standard testbed [3] to assess the scalability of our algorithms.

References

[1] V. Conitzer and T. Sandholm. Computing the optimal strategy to commit to. In *ACM Conference on Electronic Commerce*, pages 82–90, 2006.

[2] J. F. Nash. Equilibrium points in n-person games. *Proc. of the National Academy of Sciences*, 36:48–49, 1950.

[3] E. Nudelman, J. Wortman, K. Leyton-Brown, and Y. Shoham. Run the GAMUT: A comprehensive approach to evaluating game–theoretic algorithms. In *AAMAS Conference*, pages 880–887, 2004.

[4] P. Paruchuri, J. P. Pearce, J. Marecki, M. Tambe, F. Ordonez, and S. Kraus. Playing games for security: an efficient exact algorithm for solving bayesian stackelberg games. In *AAMAS Conference*, pages 895–902, 2008.

[5] B. von Stengel and S. Zamir. Leadership games with convex strategy sets. *Games and Economic Behavior*, 69:446–457, 2010.

Finding Nash Equilibria in Games With Piecewise Affine Utility Functions

Tomáš Kroupa
Università degli Studi di Milano
via Cesare Saldini 50, 20133 - Milano Italy
tomas.kroupa@unimi.it

Gaetano Vitale
Università degli Studi di Salerno
Via Giovanni Paolo II 132, 84084 Fisciano (SA) Italy
gvitale@unisa.it

Every continuous game defined over compact Hausdorff strategy spaces has a mixed Nash equilibrium by Glicksberg's theorem [1]. However, these Nash equilibria can be arbitrarily complicated Borel probability measures even if the strategy spaces are real unit intervals. Considerable research effort has been focused on identifying sufficient conditions for the existence of finitely-supported Nash equilibria. As an example of such a condition, we recall the separability of payoff functions [3]. In this contribution we make initial steps towards the problem of finding Nash equilibria for the class of constant-sum two-player games over the unit square, where the payoff functions are continuous and piecewise affine. Our method is based on the unique polyhedral subdivision of the unit square associated with the payoff function of the first player. We construct a rectangular mesh whose purpose is to sample the joint strategy space in the regions where Nash equilibria are "most likely" supported [2]. It will be shown that this algorithm recovers finite equilibria for a certain class of games and we mention several heuristics how to solve the problem in general.

References

[1] Glicksberg, I. L. A further generalization of the Kakutani fixed point theorem, with application to Nash equilibrium points. *Proceedings of the AMS*, 3:170–174, 1952.

[2] Kroupa, T., and Majer, O. Optimal strategic reasoning with McNaughton functions. *International Journal of Approximate Reasoning*, 55(6):1458–1468, 2014.

[3] Stein, N. D., Ozdaglar, A., and Parrilo, P. A. Separable and low-rank continuous games. *International Journal of Game Theory*, 37(4):475–504, 2008.

Discrete least squares polynomial approximation with random evaluations – application to PDEs with random parameters

Fabio Nobile
CSQI-MATHICSE, École Polytechnique Fédérale de Lausanne
CH-1015, Lausanne, Switzerland
fabio.nobile@epfl.ch

Albert Cohen
LJLL, Université Pierre et Marie Curie
4, place Jussieu, 75005, Paris, France.
cohen@ann.jussieu.fr

Giovanni Migliorati
LJLL, Université Pierre et Marie Curie
4, place Jussieu, 75005, Paris, France.
migliorati@ann.jussieu.fr

Raul Tempone
Applied Math. & Comput. Science, King Abdullah University of Science and Technology
4700, KAUST, Thuwal, 23955-6900, Kingdom of Saudi Arabia
raul.tempone@kaust.edu.sa

We consider a general problem $F(u, y) = 0$ where u is the unknown solution, possibly Hilbert-space valued, and y a set of uncertain parameters. We specifically address the situation in which the parameter-to-solution map $u(y)$ is smooth, however y could be very high (or even infinite) dimensional. In particular, we are interested in cases in which F is a partial differential operator, u a Hilbert-space valued function and y a distributed, space and/or time varying, random field.
We aim at reconstructing the parameter-to-solution map $u(y)$ from noise-free or noisy observations in random points by discrete least squares on polynomial spaces associated to downward closed index sets. The noise-free case is relevant whenever the technique is used to construct metamodels, based on polynomial expansions, for the output of computer experiments. In the case of PDEs with random parameters, the metamodel is then used to approximate statistics of the output quantities.
We discuss the stability of discrete least squares on random points and present error bounds both in expectation and probability for a priori chosen index sets. We will also discuss theoretical bounds on the minimal error achievable if an optimal choice of the index set for a given sample is performed among all possible downward closed index sets of given cardinality. Our theoretical bound sets a benchmark for adaptive-type algorithms that aim at discovering the optimal polynomial space.

References

[1] A. Cohen, G. Migliorati, and F. Nobile, "Discrete least-squares approximations over optimized downward closed polynomial spaces in arbitrary dimension," MATHICSE Technical Report 28.2015, École Polytechnique Fédérale de Lausanne, 2015. submitted.

[2] G. Migliorati, F. Nobile, and R. Tempone, "Convergence estimates in probability and in expectation for discrete least squares with noisy evalutations at random points," *J. Multivar. Anal.*, vol. 142, pp. 167–182, 2015.

[3] A. Chkifa, A. Cohen, G. Migliorati, F. Nobile, and R. Tempone, "Discrete least squares polynomial approximation with random evaluations – application to parametric and stochastic elliptic PDEs," *ESAIM: Math. Mod. Numer. Anal. (M2AN)*, vol. 49, no. 3, pp. 815–837, 2015.

[4] G. Migliorati, F. Nobile, E. von Schwerin, and R. Tempone, "Analysis of the discrete L^2 projection on polynomial spaces with random evaluations," *Found. Comp. Math.*, vol. 14, no. 3, pp. 419–456, 2014.

[5] G. Migliorati, F. Nobile, E. von Schwerin, and R. Tempone, "Approximation of quantities of interest in stochastic PDEs by the random discrete L^2 projection on polynomial spaces," *SIAM J. Sci. Comp.*, vol. 35, no. 3, pp. A1440–A1460, 2013.

Grouping Games: Finding Clusters in Graphs, Digraphs, and Hypergraphs

Marcello Pelillo
Università Ca' Foscari Venezia
pelillo@unive.it

Clustering refers to the process of extracting maximally coherent groups from a set of objects using pairwise, or high-order, similarities. Traditional approaches to this problem are based on the idea of partitioning the input data into a predetermined number of classes, thereby obtaining the clusters as a by-product of the partitioning process. In this talk, I'll provide a brief review of recent work done in my group which offers a radically different view of the problem. In contrast to the classical approach, in fact, we attempt to provide a meaningful formalization of the very notion of a cluster and we show that game theory offers an attractive and unexplored perspective that serves well our purpose. To this end, we formulate the clustering problem in terms of a non-cooperative *clustering game* and show that a natural notion of a cluster turns out to be equivalent to a classical (evolutionary) game-theoretic equilibrium concept. We prove that the problem of finding the equilibria of our clustering game is equivalent to locally optimizing a polynomial function over the standard simplex, and we provide a discrete-time dynamics to perform this optimization, based on the Baum-Eagon inequality. The proposed grouping framework, which has already found applications in a variety of application fields, including computer vision, security and video surveillance, bioinformatics, etc., is general and can be applied to weighted graphs, digraphs and hypergraphs alike.

References

[1] Rota Bulò, S. and Pelillo, M. 2013 *A game-theoretic approach to hypergraph clustering.* IEEE Trans. Pattern Anal. Mach. Intell. 35(6), 1312–1327.

[2] Pelillo, M. *et al.* 2013. *A game-theoretic approach to pairwise clustering and matching.* In: *Similarity-Based Pattern Analysis and Recognition* (ed. M. Pelillo). Springer, London, pp. 179–216.

Learning, games, and optimization - Part II

PROPOSERS

Roberto Lucchetti
Politecnico di Milano
Pzza Leonardo da Vinci, 32 20133 - Milano Italy
roberto.lucchetti@polimi.it

Lorenzo Rosasco
Università di Genova
Via Dodecaneso, 35 16146 Genova Italy
lrosasco@mit.edu

Silvia Villa
Istituto Italiano di Tecnologia
Via Morego, 30 16100 Genova Italy
silvia.villa@iit.it

SPEAKERS

Francisco Facchinei (keynote)
Dip. di Ing. Informatica Automatica e Gestionale, Univ. La Sapienza
facchinei@dis.uniroma1.it

Luca Calatroni
Dip. di Matematica, Univ. di Genova
calatroni@dima.unige.it

Christine De Mol
Dept. of Math. and ECARES, Univ. Libre de Bruxelles
demol@ulb.ac.be

Ernesto De Vito
Dip. di Matematica, Univ. di Genova
devito@dima.unige.it

Ilaria Giulini
INRIA Saclay Palaiseau
ilaria.giulini@inria.fr

Analytics, decision, and artificial intelligent systems have been recently revolutionized by data driven technologies fuelled with data of unprecedented size and complexity. The challenge of defining flexible models and data exploration strategies is paralleled by the need of efficiently processing big data-sets in possibly very high dimensions. The techniques to be employed arise from a combination of ideas and tools from a variety of diverse fields. Three main such fields are machine learning, game theory, and optimization. The goal of this mini-symposium is to gather experts from these fields to discuss mathematical challenges and potentially unveil novel connections.

Relevance to SIMAI The challenges of modern data driven technologies ask for new sound solutions and novel synthesis of ideas from different fields of mathematics. The mini-symposium on the "Mathematics of learning from data" we organized in the 2014 meeting had a good impact in terms of interest and audience. We believe that the proposed mini-symposium offers a unique opportunity to foster new collaborations and engage the italian applied mathematics community with the many opportunities of a new emerging field.

A parallel asynchronous lock-free algorithm for nonconvex big-data optimization

Francisco Facchinei
Università degli Studi di Roma La Sapienza
via Ariosto 25, 00185 - Roma Italy
francisco.facchinei@uniroma1.it

Loris Cannelli
Purdue University, Indiana - USA
lcannelli@purdue.edu

Vyacheslav Kungurtsev
Czech Technical University in Prague, Czech Republic
vyacheslav.kungurtsev@fel.cvut.cz

Gesualdo Scutari
Purdue University, Indiana - USA
gscutari@purdue.edu

We propose a novel *parallel asynchronous lock-free* algorithmic framework for the minimization of the sum of a smooth nonconvex function and a convex nonsmooth regularizer. This class of problems arises in many big-data applications, including deep learning, matrix completions, and tensor factorization. Key features of the proposed algorithm are: i) it deals with nonconvex objective functions; ii) it is parallel and asynchronous; and iii) it is lock-free, meaning that components of the vector variables may be written by some cores while being simultaneously read by others. Almost sure convergence to stationary solutions is proved. The method enjoys properties that improve to a great extent over current ones and numerical results show that it outperforms existing asynchronous algorithms on both convex and nonconvex problems.

Bilevel optimization for learning mixed noise models in imaging

Luca Calatroni
MIDA group, Dipartimento di Matematica (DIMA),
Università degli Studi di Genova
via Dodecaneso 35, 16146, Genova, Italy
calatroni@dima.unige.it

Carola-Bibiane Schönlieb
Department of Applied Mathematics and Theoretical Physics (DAMTP)
University of Cambridge, Wilberforce Road, CB3 0WA, Cambridge, UK
cbs31@cam.ac.uk

Juan Carlos De Los Reyes
Research Center on Mathematical Modelling (MODEMAT),
Escuela Politéecnica Nacional
Ladron De Guevara E11-253, 2507144, Quito, Ecuador
juan.delosreyes@epn.edu.ec

In this talk, we consider a PDE-constrained optimization approach to learn the optimal data model by means of training sets for some image denoising problems [1, 3]. The regularization term is fixed to be the Total Variation (TV) energy. The optimization procedure runs over two levels: the upper level, where a cost functional measuring the quality of the reconstruction is considered (examples are the L^2 norm and a smoothed version of the TV semi-norm), and the lower level, where the edge-preserving smoothing due to the TV energy is balanced against the data fitting terms by some weighting parameters to be determined throughout the optimization. After reviewing some well-posedness results, we focus in particular on the use of such strategy for learning the optimal weighting parameters in the case of the model recently proposed in [2] accounting for mixed noise distributions in a non-standard infimal-convolution fashion which allows for the decomposition of the noise into its constituent components. For an efficient and robust numerical optimization, quasi-Newton (BFGS) and Semi-Smooth Newton's approaches [4] as well as sampling strategies are used to reduce the computational costs.

References

[1] Calatroni, L. and Chung, C. and De Los Reyes, J. C. and Schönlieb, C.-B. and Valkonen, T. 2016 *Bilevel approaches for learning of variational imaging models*, in RADON book Series on Computational and Applied Mathematics, vol. 18., Berlin, De Gruyter.

[2] Calatroni, L. and De Los Reyes, J. C. and Schönlieb C.-B. 2016 *Total variation regularisation for mixed noise removal*, submitted.

[3] Kunisch, K. and Pock, T. 2012 *A bilevel optimization approach for parameter learning in variational models*, SIAM Journal on Imaging Sciences, 6(2), pp. 938-983.

[4] Lewis, A. S. and Overton, M. L. 2015 *Nonsmooth optimization via quasi-Newton methods*, Mathematical Programming Series A, 141, pp. 135-163.

Predicting Economic Time Series from Large Information Sets

Christine De Mol
Université libre de Bruxelles
Campus Plaine CPI 217, Boulevard du Triomphe, 1050 Brussels, Belgium
demol@ulb.ac.be

In our Big Data era, more and more information becomes available to predict economic variables such as inflation or gross domestic product (GDP). We discuss the problem of forecasting a given macroeconomic or financial variable, based on the information contained in a large ensemble of (stationary) time series which, typically, exhibit both serial correlation (i.e. in time) and cross-sectional correlation (i.e. between different variables). To overcome overfitting issues, the standard method proposed in the econometric literature is principal component regression [3] but other regularized regression methods such as ridge or lasso can be used as well [2]. Asymptotic consistency results can be derived for the case where both the number of time samples and the number of time series tend to infinity. We present new asymptotic rates for ridge regression, under the assumption that the series obey a so-called factor model.
An alternative to the previous strategy is to use a collection of forecasts of a given variable resulting from different sources (individual forecasters in the case of surveys, small submodels, or else different models) and to combine them linearly in order to get improved accuracy. While the common practice is to use equal combination weights, we define optimal weights that minimize the mean square forecast error in the case of point forecasts or maximize a logarithmic score in the case of density forecasts. In [1], we show that the problem is naturally regularized by the assumption that these weights are positive and sum to one and we devise simple and efficient algorithms to compute the optimal combination weights. The methodology is applied to the combination of individual forecasts of GDP and inflation from the Survey of Professional Forecasters (SPF) dataset for the Euro Area.

References

[1] Conflitti, C., De Mol, C. and Giannone, D. 2015 *Optimal combination of survey forecasts*. International Journal of Forecasting 31, 1096–1103.

[2] De Mol, C., Giannone, D. and Reichlin, L. 2008 *Forecasting using a large number of predictors: Is Bayesian shrinkage a valid alternative to principal components?* Journal of Econometrics 146, 318–328.

[3] Stock, J. H. and Watson, M. W. 2002 *Forecasting using principal components from a large number of predictors*. Journal of the American Statistical Association 97, 1167–1179.

Manifold Learning: a Reconstruction Tree Approach

Ernesto De Vito
DIMA, Università degli Studi di Genova
via Dodecaneso 35 - Genova Italy
devito@dima.unige.it

Enrico Cecini
DIMA, Università degli Studi di Genova
via Dodecaneso 35 - Genova Italy
cecini@dima.unige.it

Lorenzo Rosasco
DIBRIS, Universita' degli Studi di Genova & LCSL, M.I.T. & I.I.T.
via Dodecaneso 35 - Genova Italy
lrosasco@mit.edu

We propose and study a geometric extension of decision trees for unsupervised learning. In particular, we consider the problem of reconstructing a manifold from random samples and derive finite sample bounds depending on the intrinsic properties of the manifold. Our work is inspired by [1] and [2].

References

[1] Binev, P., Cohen, A., Dahmen, W., Devore, R. A., and Temlyakov, V. N. *Universal algorithms for learning theory part* 1*: piecewise constant functions* Journal of Machine Learning Research **6** 1297–1321 (2005)

[2] Maggioni, M., Minsker, S., and Strawn, N. *Dictionary learning and non-asymptotic bounds for geometric multi-resolution analysis* **14** 1013–1016 PAMM (2014)

Kernel Spectral Clustering

Ilaria Giulini
INRIA Saclay
1, rue Honoré d'Estienne d'Orves,
91120 Palaiseau, France
ilaria.giulini@me.com

Spectral clustering algorithms rely on the spectrum of some data-dependent matrices to perform clustering and usually a prior knowledge on the number of clusters is needed. We consider the setting of performing spectral clustering in a Hilbert space. We propose a new algorithm for spectral clustering that automatically estimates the number of classes and we study its convergence starting from an i.i.d. sample drawn according to an unknown probability distribution. The main idea is to view spectral clustering as a change of representation in a reproducing kernel Hilbert space, induced by a change of kernel. More precisely, our point of departure is the Ng, Jordan and Weiss algorithm, interpreted in a infinite-dimensional setting, where we replace the projection on the space spanned by the first eigenvectors of the Laplacian matrix with a soft truncation of the eigenvalues of the underlying integral operator. We also suggest with an example how spectral clustering, coupled with some preliminary change of representation in a reproducing kernel Hilbert space, can bring down the representation of classes to a low-dimensional space and how this approach may be used for image classification.

Model Reduction: Methods, Algorithms, Applications - Part I

PROPOSERS

Maurizio Falcone
Università La Sapienza di Roma
Piazzale Aldo Moro, 5 00185 - Roma, Italy
falcone@mat.uniroma1.it

Simona Perotto
MOX, Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano, Italy
simona.perotto@polimi.it

Gianluigi Rozza
SISSA, Area Matematica, MathLab
Via Bonomea, 265 34136 - Trieste, Italy
gianluigi.rozza@sissa.it

SPEAKERS

Yvon Maday (keynote)
Laboratoire Jacques-Louis Lions, Paris
maday@ann.jussieu.fr

Francesco Ballarin
SISSA MathLab
francesco.ballarin@sissa.it

Giulia Fabrini
Università degli Studi di Genova
giulia.fabrini@gmail.com

Luca Gerardo-Giorda
Basque Center for Applied Mathematics
lgerardo@bcamath.org

Laura Iapichino
Delft University of Technology
L.Iapichino@tudelft.nl

This minisymposium deals with recent advances in reduced order methods focusing on research current frontiers. Several topics will be presented: efficient parametrization for complex systems governed by partial differential equations, domain decomposition of parametric domains, multi-physics couplings, optimization and control, data assimilation and inverse problems, certification of accuracy, sampling techniques. Reduced order modeling is a fast growing field in applied mathematics and in computational science and engineering. It allows to face more and more complex problems with competitive computational efforts,

often in a repetitive computational settings. Among the methodologies illustrated in this minisymposium we mention proper orthogonal decomposition, reduced basis method, proper generalized decomposition and hierarchical model reduction. Applications will include continuum mechanics, like heat and mass transfer, fluid mechanics for industrial, environmental and biomedicine problems, as well as structural mechanics and material science.

Recent advances the reduced basis simulation for advection-dominated problems

Yvon Maday
Sorbonne Universités, UPMC Univ Paris 06, UMR 7598,
Laboratoire Jacques-Louis Lions, F-75005, Paris, France
IUF
Division of Applied Maths, Brown University, Providence, RI
maday@ann.jussieu.fr

Nicolas Cagniart
Sorbonne Universités, UPMC Univ Paris 06, UMR 7598,
Laboratoire Jacques-Louis Lions, F-75005, Paris, France
cagniartn@ljll.math.upmc.fr

Andrea Manzoni
dCMCS-MATHICSE-SB, Ecole Polytechnique Fédérale de Lausanne, Station 8, CH-1015 Lausanne, Switzerland
andrea.manzoni@epfl.ch

Alfio Quarteroni
dCMCS-MATHICSE-SB, Ecole Polytechnique Fédérale de Lausanne, Station 8, CH-1015 Lausanne, Switzerland
alfio.quarteroni@epfl.ch

Benjamin Stamm
Center for Computational Engineering, Mathematics Department, RWTH Aachen University, Schinkelstr. 2, 52062 Aachen, Germany
stamm@mathcces.rwth-aachen.de

Advection dominated equations is an important class of problems governed by time dependent Partial differential equations. Their numerical simulations is an important challenge for the community in numerical analysis and the class of reduced basis approximations has some difficulties to tackle these problems properly.
There are at least two reasons : the first one is due to the fact that the set of solutions (when time varies) is not with small Kolmogorov n-width — or at least does not seems so at first sight — the second is a stability issue one.
We propose here two new contributions that adresses the two issues and are explained independently in two publications [1], [2].

References

[1] Y. Maday, A. Manzoni, A. Quarteroni An online intrinsic stabilization strategy for the reduced basis approximation of parametrized advection-dominated problems, Submitted, 2016.

[2] N. Cagniart, Y. Maday, B. Stamm. in preparation, 2016.

Recent advances in reduced order modelling in computational fluid dynamics and beyond: updates on fluid-structure interaction problems

Francesco Ballarin
SISSA, International School for Advanced Studies, Mathematics Area, mathLab,
Via Bonomea 265, 34136 Trieste, Italy
francesco.ballarin@sissa.it

Gianluigi Rozza
SISSA, International School for Advanced Studies, Mathematics Area, mathLab,
Via Bonomea 265, 34136 Trieste, Italy
gianluigi.rozza@sissa.it

In this talk we will focus on recent advances in reduced order modelling for parametrized problems in computational fluid dynamics, with a special attention to the case of fluid-structure interaction problems. We will propose reduced order versions of existing numerical scheme, based either on a monolithic [1] or a segreated approach [2]. In order to handle problem on moving domains, a geometrical parametrization is introduced to deform the reference configuration into the current (time varying) configuration. Special attention will be paid to an efficient reduction of the coupling conditions. Advantages and drawbacks of reduced order monolithic vs reduced order partitioned approaches will be highlighted. Moreover, the case of a particular partioned procedure will be discussed in detailed, based on a semi-implicit operator-splitting approach. Two ROMs, which differ for the (weak vs strong) imposition of the velocity continuity coupling condition, will be discussed by means of a numerical test case, comparing the efficiency (in terms of speedup, required number of subiterations, etc.) and accuracy (with respect to the high-fidelity approach) of the proposed ROMs.

References

[1] F. Ballarin, G. Rozza. *POD–Galerkin monolithic reduced order models for parametrized fluid-structure interaction problems*. International Journal for Numerical Methods in Fluids, in press (2016).

[2] F. Ballarin, G. Rozza, Y. Maday. *Reduced-order semi-implicit schemes for fluid-structure interaction problems*. In preparation (2016).

A HJB-POD approach to the control of the level set equation

Giulia Fabrini
Università degli Studi di Genova & Laboratoire Jacques-Louis Lions, UPMC (Paris VI)
P.le Kennedy Pad. D-16129 Genova, Italy & 4 place Jussieu 75005 Paris, France
fabrini@dime.unige.it

Alessandro Alla
Florida State University, Department of Scientific Computing
400 Dirac Science Library, Tallahassee, FL 32306-4120
aalla@fsu.edu

Maurizio Falcone
Dipartimento di Matematica, Università di Roma "La Sapienza"
P. A. Moro, 5 -00185 Roma, Italy
falcone@mat.uniroma1.it

We consider an optimal control problem where the dynamics is given by the propagation of a one-dimensional graph controlled by its normal speed, which has been proposed in [3]. A target corresponding to the final configuration of the front is given and we want to minimize the cost to reach the target. We want to solve this optimal control problem via the dynamic programming approach but it is well known that this methods suffers of the "curse of dimensionality" so that we can not apply the method to the semi-discrete version of the dynamical system. However, this is made possible by a reduced-order model for the level set equation which is based on Proper Orthogonal Decomposition (see [4]). This results in a new low-dimensional dynamical system which is sufficient to track the dynamics. By the numerical solution of the Hamilton-Jacobi-Bellman equation related to the POD approximation we can compute the feedback law and the corresponding optimal trajectory for the nonlinear front propagation problem (see [1] and the reference therin for the HJB-POD approach). In particular for solving the Bellman equation we will use the accelerated policy iteration algorithm proposed in [2]. We will present some numerical tests to show the efficiency of the proposed method.

References

[1] A. Alla and M. Falcone. *An adaptive POD approximation method for the control of advection-diffusion equations*, in K. Kunisch, K. Bredies, C. Clason, G. von Winckel, (eds) *Control and Optimization with PDE Constraints,* International Series of Numerical Mathematics, **164**, Birkhäuser, Basel, 2013, 1-17.

[2] A. Alla, M. Falcone and D. Kalise. *An Efficient Policy Iteration Algorithm for Dynamic Programming Equations* SIAM J. Sci. Comput. **37** (2015), no. 1, 181-200.

[3] K. Deckelnick, C.M. Elliott, V. Styles. *Optimal control of the propagation of a graph in inhomogeneous media* SIAM J. Control. Optim. **48** (2009), no. 3, 1335-1352.

[4] S. Volkwein. *Model Reduction using Proper Orthogonal Decomposition*, Lecture Notes, University of Konstanz, 2011

Model reduction for the dispersal of invasive species in a realistic landscape

Luca Gerardo-Giorda
BCAM – Basque Center for Applied Mathematics
Alameda Mazarredo 14, E-48009 Bilbao, Spain
lgerardo@bcamath.org

Francesco Montomoli
Department of Aeronautics
Imperial College London
South Kensington Campus, London SW7 2AZ, UK
f.montomoli@imperial.ac.uk

Invasive species can be a major threat for an ecosystem, and have been subject of several studies in the ecological community. In addition, contrasting exogenous agents can take a serious toll to the annual budget of Departments of Environmental Protection. Accurate mathematical models can be efficient predictive tools on which building a proper intervention strategy, but their development faces some nontrivial difficulties. One of the main difficulties in simulating the spread of an invasive species (animal or plant) in wildlife resides in properly taking into account the heterogeneities of the landscape [1]. Another major difficulty resides in the poor knowledge of the characterising parameters of the population dynamics itself, such as reproductive rate, carrying capacity of the environment, and dispersal speed. A direct approach to cope with this uncertainty is the Monte Carlo Method (MCM), a robust, flexible, and non-intrusive approach. As MCM does not impose any restriction on the distributions of the input parameters, distributions with fat tails that increase the frequency of occurrence for black-swan events can easily be used. However, MCM is characterised by a slow convergence rate, as it relies on sampling the stochastic space of parameters to perform a large amount of independent deterministic simulations. The use of MCM coupled with meta-models significantly improves the speed of the method. Meta-models rely on a limited number of deterministic simulations and suitable interpolation techniques such as Kriging to identify a response surface for Quantities of Interest, whose computation is the actual objective of the MCM. The convergence rate is always $1/\sqrt{N}$, but the extremely fast computation for each parameter sample allows to increase the number of Monte Carlo samples ad libitum. We will introduce the MCM with meta-models technique and show the effectiveness of our method in the dispersal of a generic exogenous agent in the region of the Basque Country.

References

[1] L. Gerardo-Giorda and F. Montomoli (2016) *High detail geographical modeling of the dispersal of invasive species* (submitted)

[2] L. Gerardo-Giorda and F. Montomoli (2016) *A metamodel approach to the dispersal of invasive species* (in preparation)

Reduced Basis methods for PDE Constrained Multi-objective Optimization

Laura Iapichino
Delft University of Technology
Mekelweg 5, 2628 CC Delft, The Netherlands
l.iapichino@tudelft.nl

Stefan Trenz
Politecnico di Milano
University of Konstanz
Universitätsstraße 10, D-78457 Konstanz, Germany
stefan.trenz@uni-konstanz.de

Stefan Volkwein
University of Konstanz
Universitätsstraße 10, D-78457 Konstanz, Germany
stefan.volkwein@uni-konstanz.d

Problems where several objective functions have to be simultaneously optimized, often arise in many applicative contexts. Compared with optimal control problems with a single objective functions, multiobjective problems are more complex and require longer computational times to be solved. Reduced order techniques for the numerical solution of multiobjective optimization with linear and semilinear PDEs constraints are proposed. The aim is to find solutions in reasonable computational times which do not penalize the optimization of any objective function and which represent a good compromises for all the individual ones. In general, does not exist a single optimal solution, but there exists a (possibly infinite) number of optimal solutions, called Pareto points. In the multiobjective optimization theory, the Pareto optimality allows to determine efficient optimal points for all the considered objective functions [1]. We apply the reduced basis method [2] in this context to handle the computational complexity and resolution times of the problem and, at the same time, to ensure a suitable level of the solution accuracy.

References

[1] C. Hillermeier. Nonlinear multiobjective optimization. A generalized homotopy approach. Birkhaeuser Verlag, Basel, 2001

[2] J. S. Hesthaven, G. Rozza, B. Stamm. Certified Reduced Basis Methods for Parametrized Partial Differential Equations. Springer. 2016

Model Reduction: Methods, Algorithms, Applications - Part II

PROPOSERS

Maurizio Falcone
Università La Sapienza di Roma
Piazzale Aldo Moro, 5 00185 - Roma, Italy
falcone@mat.uniroma1.it

Simona Perotto
MOX, Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano, Italy
simona.perotto@polimi.it

Gianluigi Rozza
SISSA, Area Matematica, MathLab
Via Bonomea, 265 34136 - Trieste, Italy
gianluigi.rozza@sissa.it

SPEAKERS

Wil H.A. Schilders (keynote)
TU Eindhoven
w.h.a.schilders@tue.nl

Angelo Iollo
University of Bordeaux
Angelo.Iollo@math.u-bordeaux1.fr

Laura Mainini
Massachusetts Institute of Technology
lmainini@mit.edu

Alessio Spantini
Massachusetts Institute of Technology
spantini@mit.edu

Dante Kalise
Johann Radon Institute for Computational and Applied Mathematics (RICAM)
dante.kalise@oeaw.ac.at

This minisymposium deals with recent advances in reduced order methods focusing on research current frontiers. Several topics will be presented: efficient parametrization for complex systems governed by partial differential equations, domain decomposition of parametric domains, multi-physics couplings, optimization and control, data assimilation and inverse problems, certification of accuracy, sampling techniques. Reduced order modeling is a fast growing field in applied mathematics and in computational science and engineering. It allows to face more and more complex problems with competitive computational efforts,

often in a repetitive computational settings. Among the methodologies illustrated in this minisymposium we mention proper orthogonal decomposition, reduced basis method, proper generalized decomposition and hierarchical model reduction. Applications will include continuum mechanics, like heat and mass transfer, fluid mechanics for industrial, environmental and biomedicine problems, as well as structural mechanics and material science.

A MOR method to speed up the simulation of highly nonlinear oscillatory electronic circuits

Wil H.A. Schilders
TU Eindhoven,
Centre for Analysis, Scientific Computing and Applications,
The Netherlands

G. De Luca
TU Eindhoven,
Centre for Analysis, Scientific Computing and Applications,
The Netherlands

The electronics industry has always been one of the most stimulating environments for techniques in the area of model order reduction. Starting with the advent of AWE, and the subsequent development of PVL, PRIMA and other methods, one always encounters examples from the electronics industry, more specifically for device and circuit simulation. Although slowly but steadily other application domains are entering the field, the electronics industry remains a prime source for challenges in model order reduction. Especially for nonlinear and highly oscillatory circuits, there is a big challenge, as simulation times are often a few days or even weeks, and this is not acceptable for designers. What's more, when looking at the solutions generated in the time domain, one gets the feeling that it should be possible to model the behaviour in a more concise and compact way, as solutions only change very slowly from one period to another. However, how to capture this slowly changing behaviour is a challenge in itself. Initially, we have been thinking of applications of (D)EIM or POD, but so far the attempts were not successful. An important case of so-called quasi-periodic circuits with very long simulation time are phaselocked loops (PLLs). PLLs find their applications in wireless systems, digital circuits and medical devices. Time domain analyses are performed by numerically integrating the circuit's DAEs. For PLLs, the time step during integration is related to the PLL's output frequency f_{out}, which is often in the GHz range, meaning that a huge number of steps will be made. Designers simulate PLLs for a large period of time to extract important characteristics such as power consumption, locking time, phase noise and jitter. Previous work on speeding up the simulation of PLLs is based on partial or full replacement of PLL blocks by macromodels, others use full TL simulation (e.g., see [1, 2, 3]). However, none of them estimates all the PLL characteristics very well. In fact, promising initial work was done in the 1990's, but necessary improvements to truly speed up simulations were not found. We propose a technique to accurately extract all the aforementioned characteristics of PLL's while very substantially accelerating noise-free and noisy simulations, by replacing only the VCO and divider blocks in the PLL with a single phase macromodel, built through steady-state (SST) analyses [4, 5] and SST noise methods [6, 7] The method leads to a reduced order model for the full PLL. The methodology is applicable to other types of highly nonlinear and osciallatory devices, and we will also indicate future work on such devices that are even more challenging.

References

[1] P. Maffezzoni and S. Levantino, Analysis of VCO phase noise in charge-pump phase-locked loops. *IEEE Trans. Circuits Syst. I: Regular Papers* , vol. 59, n. 10, pp. 2165-2175, 2012.

[2] X. Lai and J. Roychowdhury, TP-PPV: piecewise nonlinear, time-shifted oscillator macromodel extraction for fast, accurate PLL simulation. *ICCAD*, Hassoun, Soha, 2006.

[3] K. Bittner and H. G. Brachtendorf, Adaptive multi-rate wavelet method for circuit simulation. *Radioengineering*, vol. 23, pp. 300-307, 2014.

[4] K. S. Kundert and A. Sangiovanni-Vincentelli, Finding the steady-state response of analog and microwave circuits. *Proceedings of the IEEE on Custom Integrated Circuits Conference*, pp. 6.1/1-6.1/7, 1988.

[5] R. Telichevesky, K. S. Kundert and J. K. White, Efficient Steady-State Analysis Based on Matrix-Free Krylov-Subspace Methods. *32nd Design Automation Conference (DAC)*, pp. 480-484, 1995.

[6] E. Ngoya, J. Rousset and D. Argollo, Rigorous RF andmicrowave oscillator phase noise calculation by envelopetransient technique. *IEEE MTT-S International Microwave Symposium Digest.*, vol. 1, pp. 91-94, 2000.

[7] A. Demir, A. Mehrotra and J. Roychowdhury, Phase noise in oscillators: a unifying theory and numericalmethods for characterization. *IEEE Trans. Circuits Syst. I*, vol. 47, pp. 655-674, 2000.

Monge-Kantorovich Interpolation for PDE Constrained Optimization

Angelo Iollo
Université de Bordeaux and Inria Bordeaux - Sud Ouest
351, cours de la Libération Talence, France
angelo.iollo@inria.fr

Michel Bergmann
Université de Bordeaux and Inria Bordeaux - Sud Ouest
351, cours de la Libération Talence, France
michel.bergmann@inria.fr

Haysam Telib
Optimad Engineering srl
via Giacinto Collegno 18 - Torino Italy
haysam.telib@optimad.it

Classical model reduction techniques approximate the solution of a physical model by a limited number of global modes. However, when the physics of the model is mainly characterized by advection, the non-local representation of the solution by global modes essentially reduces to a Fourier expansion. Principal Component Analysis (PCA) is the main tool behind many techniques to perform model reduction of systems of partial differential equations (PDEs). The principle of PCA is to find a global base of a small dimensional subspace in such a way that the solution of a given PDE is accurately represented in this subspace. This is the main idea behind Proper Orthogonal Decomposition (POD) [4]: POD extracts a basis that minimizes the L^2 average distance between the reduced representation and a solution database. POD approximations are usually satisfactory for those problems where the solution has a global behavior or is periodic [1, 2], but perform poorly for systems characterized by concentrated structures that are mapped as a function of parameter variations. The main reason for this is that a simple shift cannot be represented by a finite linear combination of global modes. The reduced basis method [6] is another global mode approach alternative to POD, with a rigourous mathematical setting for certain classes of elliptic or parabolic problems. Alternatives to POD taking implicitly into account the notion of transport in the definition of a global reduced basis are provided by Koopman modes [7] and Dynamic Mode Decomposition (DMD) [8]. These approaches assume the existence of a linear propagator whose spectrum provides a frequency-based mode decomposition of the considered evolution. Other authors derive specific modes for the advection operator via a greedy collocation algorithm [3]. Our objective is different. We introduce the notion of advection modes: when advection is the leading phenomenon, a hierarchy of advection modes can adequately approximate the mapping of coherent structures. The advection modes can be found based on the solution of Monge-Kantorovich mass transfer problems as in [5]. Examples pertaining to unsteady compressible flows will be presented.

References

[1] M. Bergmann, C.H. Bruneau, and A. Iollo. *Enablers for robust pod models*. JCP, 228:516–538, 2009.

[2] Galletti, C. H. Bruneau, L. Zannetti, and A Iollo. *Low-order modelling of laminar flow regimes past a confined square cylinder*. JFM, 503:161–170, 1999.

[3] M. A. Grepl, Y. Maday, N.C. Nguyen, and A. T. Patera. *Efficient reduced-basis treatment of non-affine and nonlinear partial differential equations*. Math. Model. Numer. Anal., 41:575–605, 2007.

[4] P. Holmes, J.L. Lumley, and G. Berkooz. *Turbulence, coherent structures, dynamical systems and symmetry*. Cambridge University Press, 1st edition, 1996.

[5] A. Iollo and D. Lombardi. *Advection modes by optimal mass transfer*. PRE, 89(2):022923, February 2014.

[6] A. Manzoni, A. Quarteroni, and G. Rozza. *Shape optimization for viscous flows by reduced basis methods and freeform deformation*. International J. Num. Meth. in Fl., 70:646–670, 2012.

[7] I. Mezic. *Spectral properties of dynamical systems, model reduction and decompositions*. Nonlinear Dyn., 41:309–325, 2005.

[8] P. Schmid. *Dynamic mode decomposition of numerical and experimental data*. JFM, 656:5–28, 2010.

A Reduced Order Modeling Strategy for Real Time Structural Assessment from Sparse Measurements

Laura Mainini
Massachusetts Institute of Technology
77 Massachusetts Avenue, Cambridge, MA, 02139-4307, USA
lmainini@mit.edu

Next generations of transportation systems will be able to autonomously develop operative strategies in real time, taking into account the evolution of their health condition along with the dynamic changes of the surrounding environment. A practical example is the case of autonomous aerospace vehicles that dynamically adapt their mission to the evolution of their structural state. For problems of this kind, a first challenge is the limited time and resources that can be dedicated on board to data processing; in addition, cost and weight of state-of-the-art sensing technologies represent another relevant constraint and motivate the development of strategies to optimize sensors placement. Finally, both onboard measurements and inference from sparse sensor data introduce uncertainties that can potentially affect the overall data to decisions process.
In previous works [1, 2] we proposed to write this class of problems in the form of a sense-infer-plan-act information flow associated to two distinct sets of quantities of interest: measured quantities of interest and capability quantities of interest. Measurements are physical quantities that can be monitored with sensors (e.g. strain components) and represent the source of information about the state of a system (e.g. damage condition); capabilities (e.g. failure indices) are quantities that dynamically evolve with the state of a system and limit the space of possible actions. Then, we tackled the specific time-critical problem of estimating capabilities from measurements. Our methodology relies on an offline-online approach and combines reduced order modeling, data-fit surrogate modeling, and clustering techniques into a multistep flexible computational framework.
This talk illustrates our offline-online approach for an aerospace structural application involving a damage assessment problem. The particular implementation adopts parametric proper orthogonal decomposition to obtain the first reduction, self-organizing maps to achieve model localization, and polynomial response surfaces to build localized models that map from measured data to system capabilities. The discussion focuses on our extensive investigations and recent improvements for the case of sparse sensor measurements affected by uncertainties. We present tuning strategies to obtain rapid and effective capability evaluations accounting for measurements uncertainty. Along with the relevant time savings, our studies demonstrate the possibility to achieve normalized root mean square errors of about 6%, 1.5% and 1.3% in predicting capabilities from incomplete onboard measurements that present 95%, 80% and 50% of missing data, respectively.

References

[1] Mainini, L. and Willcox, K. 2015 Surrogate modeling approach to support real-time structural assessment and decision making. *AIAA Journal*. Vol. 53, No. 6, 1612–1626.

[2] Mainini, L. and Willcox, K. 2015 Sensitivity analysis of surrogate-based methodology for real-time structural assessment. AIAA Paper 2015-1362. *AIAA SciTech 2015*, Kissimmee, FL, January 5-9, 2015.

Measure transport, inference and low-dimensional maps

Alessio Spantini
Massachusetts Institute of Technology
Cambridge, MA, 02139, USA
spantini@mit.edu

Daniele Bigoni
Massachusetts Institute of Technology
Cambridge, MA, 02139, USA
dabi@mit.edu

Youssef Marzouk
Massachusetts Institute of Technology
Cambridge, MA, 02139, USA
ymarz@mit.edu

A recent approach to non-Gaussian Bayesian inference seeks a deterministic transport map that pushes forward a reference density to the posterior. In this talk, we address the computation of transport maps in high dimensions. In particular, we show how the Markov structure of the posterior density induces low-dimensional parameterizations of the transport map. Topics include the sparsity of inverse triangular transports, the ordering of the Knothe-Rosenblatt rearrangement, decompositions of transports, and other related ideas in dimensionality reduction for Bayesian inversion.

Optimal feedback control of reduced-order semilinear parabolic equations

Dante Kalise
Johann Radon Institute for Computational and Applied Mathematics (RICAM)
Altenbergerstraße 69, 4040 Linz, Austria
dante.kalise@oeaw.ac.at

Karl Kunisch
University of Graz
Universitätsplatz 3, 8010 Graz, Austria
karl.kunisch@uni-graz.at

Feedback control design plays a fundamental role in modern engineering. For an optimality-based formulation of the control problem, the Dynamic Programming Principle allows the characterization of the associated value function as the viscosity solution of a first-order, fully nonlinear Hamilton-Jacobi-Bellman equation. The equation is defined over the state-space of the controlled dynamical system and therefore, even control problems over low-dimensional dynamics lead to HJB equations of high complexity. In this talk, we present an approximation framework to compute (sub)optimal feedback controllers based on the solution of a Generalized HJB equation and a policy iteration algorithm. The controller is computed upon a state space representation of reduced dimension, obtained via spectral elements. Problems arising from the feedback control of partial differential equations illustrate the effectiveness of our approach in a high-dimensional context.

References

[1] D. Kalise and K. Kunisch. *An spectral element method for Hamilton-Jacobi-Bellman equations*, in preparation.

[2] D. Kalise, A. Kröner and K. Kunisch. *Local minimization algorithms for dynamic programming equations*, to appear in SIAM Journal on Scientific Computing.

[3] O. Bokanowski, M. Falcone, R. Ferretti, L. Grüne, D. Kalise and H. Zidani. *Value iteration convergence of ϵ-monotone schemes for stationary Hamilton-Jacobi equations*, Discrete and Continuous Dynamical Systems - Series A **35**(9)(2015), 4041–4070.

[4] A. Alla, M. Falcone and D. Kalise. *An efficient policy iteration algorithm for the solution of dynamic programming equations*, SIAM Journal on Scientific Computing **37**(1)(2015), 181–200.

Computational Optimization and Applications

PROPOSERS

Valeria Ruggiero
Università di Ferrara
rgv@unife.it

Gerardo Toraldo
Università degli Studi di Napoli Federico II
gerardo.toraldo@unina.it

SPEAKERS

Daniela Lera
Dip. di Matematica e Informatica, Università di Cagliari
lera@unica.it

Benedetta Morini
Dip. di Ingegneria Industriale, Università di Firenze
benedetta.morini@unifi.it

M. Flavia Monaco
Dip. di Ingegneria Informatica, Modellistica, Elettronica e Sistemistica, Università della Calabria
monaco@dimes.unical.it

Daniela di Serafino
Dip. di Matematica e Fisica, Seconda Università di Napoli
daniela.diserafino@unina2.it

Riccardo Pellegrini
Università di Roma 3, Dip. di Ingegneria. Via Vito Volterra 62, Rome, Italy,
riccardo.pellegrini@uniroma3.it

Stefania Bellavia
Dip. di Ingegneria Industriale, Università di Firenze
stefania.bellavia@unifi.it

Computational optimization is an important paradigm with a wide range of applications in engineering design and control, computational chemistry, computer science, industry, economics and management [1, 2]. In many cases, the search for optimality is challenging, either because of the high computational cost of evaluating objectives and constraints, or because of the nonlinearity, multimodality, discontinuity and uncertainty of the problem functions in the real-world systems.
The aim of this minisymposium is to provide some recent advances in computational optimization, that lead to novel techniques for local and global minimization, and for the solution of systems of nonlinear equalities and inequalities. The algorithms are especially tuned to address significant applications arising from different domains, such as the

shape-from-shading technique (in computer vision), the management of logistic processes, the design of complex engineering systems.

References

[1] Yang, X. S. and Koziel, S. 2011 *Computational Optimization and Applications in Engineering and Industry*, Studies in Computational Intelligence, Springer-Verlag, Berlin.

[2] Chandra, S., Jayadeva and Aparna, M. 2009 *Numerical Optimization with Applications*, Alpha Science Intl Ltd

The Global Minimization Problem Using Space-filling Curves

Daniela Lera
Università degli Studi di Cagliari
via Ospedale, 72 09124 - Cagliari Italy

Yaroslav Sergeyev
Università della Calabria
via P. Bucci, Cubo 42-C 87036 - Rende (CS) Italy
Lobachevsky State University of Nizhni Novgorod, Russia
yaro@dimes.unical.it

Many decision-making problems arising in various fields of human activity (technological processes, economic models, etc.) can be stated as global optimization problems (see, e.g., [1, 2, 3, 8, 10]). An interesting application is, for example, that of the detection of the first zero-crossing in a measurement signal set [7]. This problem arises in the non-parametric identification of special signals, in the Wavelet transform and image processing [6, 11]. Objective functions describing real-life applications are very often multiextremal, nondifferentiable, and hard to evaluate. Numerical techniques for finding solutions to such problems have been widely discussed in the literature (see, e.g., [9, 10]). In this talk, the Lipschitz global optimization problem is considered.
Mathematically, the global optimization problem considered in the paper can be formulated as minimization of a multidimensional multiextremal "black-box" function that satisfies the Lipschitz condition over a domain $[a, b] \subset R^N$ with an unknown constant L, i.e., finding the value F^* and points y^* such that

$$F^* = F(y^*) = \min\{F(y) : \ y \in [a, b]\}, \tag{1}$$

$$|F(y') - F(y'')| \leq L\|y' - y''\|, \qquad y', y'' \in [a, b], \tag{2}$$

with a constant L, $0 < L < \infty$. To attack the problem we consider the following two ideas. First, an approach that uses numerical approximations of space-filling curves to reduce the original Lipschitz multi-dimensional problem to a univariate one satisfying the Hölder condition [4, 9] is applied.
Second, we propose several techniques for acquiring the Hölder information that can be distinguished with respect to the way the Hölder constant is estimated during the process of optimization. In particular, we consider techniques that use either a global estimate of the Hölder constant valid for the whole search region, or local estimates H_i valid only for some subregions of the domain [4]. Moreover, a new geometric technique working with a number of possible Hölder constants chosen from a set of values varying from zero to infinity is considered showing so that ideas introduced in a popular DIRECT method can be used in the Hölder global optimization [5].

Acknowledgements The research of Ya.D. Sergeyev was supported by the Russian Science Foundation, project No 15-11-30022 "Global optimization, supercomputing computations, and applications".

References

[1] Carotenuto L., Pugliese P., Sergeyev Ya.D. 2006 *Maximizing performance and robustness of PI and PID controllers by global optimization.* Control Intell. Syst. 34(3), 225–235.

[2] Floudas C.A., Pardalos P.M., Adjiman C., Esposito W., Gümüs Z., Harding S., Klepeis J., Meyer C., and Schweiger C. 1999 *Handbook of Test Problems in Local and Global Optimization.* Kluwer Academic Publishers, Dordrecht, The Netherlands.

[3] Kvasov D.E., Menniti D., Pinnarelli A., Sergeyev Ya.D., Sorrentino N. 2008 *Tuning fuzzy power-system stabilizers in multi-machine systems by global optimization algorithms based on efficient domain partitions.* Electr. Pow. Syst. Res. 78, 1217–1229.

[4] Lera D., Sergeyev, Ya.D. 2013 *Acceleration of univariate global optimization algorithms working with Lipschitz functions and Lipschitz first derivatives.* SIAM J. Optim. 23(1), 508–529.

[5] Lera D., Sergeyev Ya.D. 2015 *Deterministic global optimization using space-filling curves and multiple estimates of Lipschitz and Hölder constants.* Commun. Nonlinear Sci. Numer. Simul. 23, 328–342.

[6] Mallat S. 1991 *Zero crossing of a wavelet transform.* IEEE Trans. Inform. Theory 37(4), 1019–1033.

[7] Molinaro A., Sergeyev, Ya.D. 2001 *An efficient algorithm for the zero crossing detection in digitized measurement signal.* Measurement 30, 187–196.

[8] Pintér, J. 1996 *Global Optimization in Action (Continuous and Lipschitz Optimization Algorithms, Implementations and Applications).* Kluwer Academic Publishers, Dordrecht, The Netherlands.

[9] Sergeyev Ya.D, Strongin R.G., Lera D. 2013 *Introduction to Global Optimization Exploiting Space-Filling Curves.* Springer, New York.

[10] Strongin R.G., Sergeyev Ya.D. 2000 *Global Optimization with Non-convex Constraints: Sequential and Parallel Algorithms.* Kluwer Academic Publishers) Dordrecht, The Netherlands.

[11] Zackar A., Oppenheim A.V. 1990 *Reconstruction of two dimensional signals from level crossing.* Proc. of the IEEE 78(1), 31–35.

On the solution of constrained nonlinear systems with applications to gas distribution networks

Benedetta Morini
Università degli Studi di Firenze
viale Morgagni, 40 50134 - Firenze Italy
benedetta.morini@unifi.it

Leopoldo Marini
Università degli Studi di Firenze
via di S. Marta 3 50139 - Firenze Italy
leopoldo.marini@unifi.it

Margherita Porcelli
Università degli Studi di Firenze
viale Morgagni, 40 50134 - Firenze Italy
margherita.porcelli@unifi.it

Systems of nonlinear equations subject to constraints model a variety of applications, such as oil and gas extraction, gas transportation and distribution. The dimension of such systems varies widely among the applications considered.
The numerical solution of constrained systems has been intensively investigated in the last years. Most of the proposed methods require the calculation of partial derivatives of the nonlinear mapping and are Newton-based procedures. On the other hand, in medium and large scale problems, iterations may be burdensome unless the Jacobian matrix is structured and proper computations reduce the computational effort. Whenever computing derivatives and solving the linear algebra phase arising at each iteration is costly, Quasi-Newton methods may become competitive. Interestingly, suitable implementations of Quasi-Newton methods do not involve derivatives at all.
In this talk we present a new Quasi-Newton method for constrained nonlinear systems. Throughout the iterative process, both the computation of the trial steps and the globalization strategy are performed without requiring derivatives of the nonlinear mapping. We discuss the theoretical properties of the proposed approach and different implementations. Experimental results on problems from the literature and on gas distribution networks are presented.

Optimization problems in the operational management of a container terminal

M. Flavia Monaco
Università della Calabria
via P. Bucci 44, 87036 - Rende (CS) Italy
monaco@dimes.unical.it

Manlio Gaudioso
Università della Calabria
via P. Bucci 44, 87036 - Rende (CS) Italy
gaudioso@dimes.unical.it

Marcello Sammarra
ICAR - CNR
via P. Bucci 7-11 C, 87036 - Rende (CS) Italy
sammarra@icar.cnr.it

The sea world trade and, in particular, that of containerized cargo, has steeply increased in the last decades. Therefore, transshipment container terminals (hubs) are become the most relevant nodes in the worldwide transportation network. A transshipment port is a very complex system, where daily a large number of processes need to be optimized, and the related terminal resources coordinated, in order to guarantee valuable rates of efficiency. Therefore the terminal managers have to face the increasing freight volumes, the handling of always larger containerships, while efficiently managing the available resources (equipment and manpower) and the related logistic processes. Although the decision making process is usually hierarchical, which leads to tackle each managerial problem on separate and independent stages, problems still remain very difficult to solve. Actually most of them are modeled as Integer Linear Programs, characterized by a huge number of decision variables and constraints. For this reason they represent a challenging task for standard optimization methods: commercial solvers embedding classical algorithms often fail also in computing feasible solutions in a reasonable amount of time.
We briefly survey the most significant optimization problems arising in the management of a transshipment container terminal at the operational level. In particular we refer to the Gioia Tauro Container Terminal, one of the most important hub ports in the Mediterranean Sea. Some of these problems have been extensively studied in the scientific literature: we outline our point of view and the contribution of our past research to their solution [3]. Then we focus on some new problems which are the object of our current research.

Terminal operations and decision problems

The main activity of a transshipment container terminal consists in loading/unloading containers into/from vessels, by means of quay cranes. The decision problems originating from this basic process can be individuated and grouped in relation to the flow of containers

inside the terminal. Containers enter and leave the terminals by means of containerships. Therefore the first decision concerns *where* and *when* a containership has to be berthed along the quay. This is the *Berth Allocation Problem*. Here different optimality criteria can be used. However, the (weighted) sum of the time the containerships spend in port is widely adopted (turnaround time) [2].
Once a containership is moored at the quay, the discharging/loading process of containers can effectively start. To optimize this process, the terminal planners have to decide the number of quay cranes to allocate to the containership, and the sequence of containers each quay crane has to handle. This is the *Quay Crane Assignment and Scheduling Problem* [1]. In this problem it is quite obvious to minimize the time when the last operation on the containership is executed (*makespan*). Closely related to the Quay Crane Assignment and Scheduling Problem is the *Ship Stowage Planning Problem*, that is to decide how the export containers have to be placed within the containership, assuming to be given the sequence of containers handled by the quay cranes, in order to minimize the terminal operative costs [5]. The above described problems pertain to the so called *quay-side operation planning*.
A second group of problems constitute the *transport operation planning*, where the movements of containers between the quay and the yard must be decided. This category of problems strictly depend on the particular terminal one considers, that is on the equipment used and on the layout and organization of the yard. Gioia Tauro has large storage spaces, where stacks are up to four containers high, and uses mobile cranes called straddle carriers. They are machines capable to transport (and stack) one or two twenty-feet containers. The wideness of the space where the straddle carriers operate and the limited transport capacity call for optimizing the distance they travel in moving containers between the yard and the quay, in particular the distance to reach the next container to be moved (*empty travels*) [3].
The third and last group of problems concern the *yard logistics*, that includes all the decision problems related to the planning of the storage spaces. Here the objectives are mainly oriented at attaining a fast retrieval of the export containers and to maintain the stacking spaces as de-fragmented as possible. This is achieved by deciding *where* import containers have to be allocated and *where* and *when* the stored containers have to be eventually reallocated, in order to make room for the forthcoming containers [3].
In closing this brief review one has to consider that the container handling is executed by means of *manned* machines. Therefore there are always human operators to be considered when the operations of the terminal are planned. The *Manpower Planning Problem* at a container terminal concerns the ground crew, that is, workers (drivers, checkers, deck-men, risers) involved in the activities related to loading/discharging operations, as well as to the handling of containers on the yard [3].
It is worthy to underline that the above described problems depend on each other, although we have described them as stand-alone problems. As an example one has just to observe that the time a containership spends in port depends on:

1. the number of quay cranes allocated to its handling, and on the stowing position of the containers;

2. the distance between the berth and the yard block where the import containers must be stacked (or the export containers are stored);

3. the number of workers involved in the loading/dischargin operations.

New research trends

Direct Transshipment Transshipment container terminals are characterized by a bidirectional flow of containers: containers discharged from a vessel are usually stored in the yard, and then loaded on different vessels. The storage phase allows to decouple in time the import and export container flows. Therefore, if the sojourn time of the containers (dwell-time) in the yard is sufficiently long, the discharging and loading operations are independent, so that they can be planned and scheduled separately and efficiently. On the other hand, high dwell-times represent a drawback for the terminal management as well as for the shipping operators. Actually the former would increase the terminal throughput by reducing the dwell-times, and the shipping operators would reduce the port fees. This amounts to say that short dwell-times is a common target for the two main operators of the transshipment market. In view of that, the terminal planners are considering the feasibility of a new operational modality, called *Live Connection*. In this modality a discharged container is immediately transshipped to the outgoing vessel, completely skipping the yard storage phase. Here we are concerned with the case of two vessels, simultaneously berthed at not necessarily adjacent berths, given that sufficient terminal resources (machines and operators) have been previously allocated. We assume that some of the containers discharged from each of them must be directly loaded into the other, while the rest of the cargo follows the conventional transshipment flow (quay-yard-quay). In the direct transshipment modality the unloading and loading operations are no longer independent and the related scheduling processes are concurrent: the same container represents two dependent tasks, to be executed by different machines (quay cranes) operating on different vessels, linked by a strict precedence relationship. Clearly the stowing position of the containers directly transshipped to the export vessel is unknown. Thus the aim is to schedule all the vessel operations and decide the stowage positions for the containers directly transshipped, so as to minimize their waiting time and the overall service time of the vessels. For this problem we present a Linear Integer model proposed in [4], describe some advances in the solution procedure based on the Tabu Search paradigm and discuss the numerical experience.

Maintenance Planning There is a wide agreement on the fact that the reliability and availability of the cargo handling equipment play a very relevant role to guarantee a high quality service. Actually, the most significant indicators of the global terminal performance (throughput, turnaround time) are related to the vessel service time, which, on turn, is strongly influenced by the continuous availability and full functionality of the technical resources. Nevertheless, the planning and management of the equipment repair and maintenance has not received, so far, enough attention in the scientific literature.
In order to introduce the problem, it is worthy to underline that most of the maintenance activities require the downtime of the involved equipment; therefore it is not easy to allocate suitable servicing time windows without affecting the terminal operative continuity. For this reason, the planning of the maintenance activities follows a two-phase process. On the basis of the weekly berthing plan, the service records and the forthcoming deadlines for the preventive maintenance activities of the equipment, the first phase (long-term planning) is aimed at selecting the equipment to inspect. Then, given the set of equipment to be serviced, the second phase (short-term planning) consists of scheduling all the maintenance activities, while taking into account the availability of the workers responsible for the maintenance.
Here we describe an optimization model for the periodic preventive maintenance of the

container handling equipment. Inspired by the real context of the Gioia Tauro container terminal, we discuss the problem, and focus on the short-term planning problem. Some preliminary numerical results on real instances are presented.

References

[1] Moccia, L. and Cordeau, J.-F. and Gaudioso, M. and Laporte, G. 2006. *A branch-and-cut algorithm for the quay crane scheduling problem in a container terminal*. Naval Research Logistics. 53(1) 2006, 45 - 59.

[2] Monaco, MF. and Sammarra, M. 2007. *The berth allocation problem: a strong formulation solved by a Lagrangean approach*. Transportation Science. 41 (2), 2007, 265 - 280.

[3] Monaco, MF. and Moccia, L. and Sammarra, M. 2009. *Operations research for the management of a transhipment container terminal: the Gioia Tauro case*. Maritime Economics & Logistics. 11(1) 2009, 7-35.

[4] Monaco, MF. and Sammarra, M. 2012. The Direct Ship-to-Ship Container Transshipment Problem at a Maritime Container Terminal. In *Proceedings of the 2012 International Conference on Logistics and Maritime Systems - LOGMS2012*. Gunther H.-O., Kim K.-H., and Kopfer H. (Eds). pp. 79-89.

[5] Monaco, MF. and Sammarra, M. and Sorrentino, G. 2014 *The terminal-oriented ship stowage planning problem*. European Journal of Operational Research 239 (1), 2014, 256 - 265.

Two-phase gradient algorithms for quadratic programming problems with a single linear constraint and bounds on the variables

Daniela di Serafino
Seconda Università degli Studi di Napoli
viale A. Lincoln 5, 81100 Caserta, Italy
daniela.diserafino@unina2.it

Gerardo Toraldo
Università degli Studi di Napoli Federico II
via Cintia, 80126 Napoli, Italy
toraldo@unina.it

Marco Viola
Università degli Studi di Roma La Sapienza
via Ariosto 25, 00185 Roma, Italy
marco.viola@uniroma1.it

We propose an algorithmic framework for the solution of Quadratic Programming problems with a Single Linear equality constraint and lower and upper Bounds (SLBQP problems):

$$\begin{aligned} \min \quad & \frac{1}{2} x^T H\, x - c^T x, \\ \text{s.t.} \quad & l \leq x \leq u, \\ & a^T x = b, \end{aligned}$$

where $H \in \mathbb{R}^{n \times n}$ is symmetric positive definite, $a, c, l, u \in \mathbb{R}^n$ and $b \in \mathbb{R}$. Problems of this type arise in many applications, e.g. Support Vector Machine training, portfolio selection, multicommodity network flow and logistics [4, 6, 7]. Furthermore, SLBQP problems can be regarded as "building blocks" for the solution of some more general nonlinear constrained problems.
Inspired by the GPCG method [5] for bound-constrained quadratic programming, the algorithms in our framework alternate between two phases until convergence:

- an *identification phase*, which performs Gradient Projection iterations, using Barzilai-Borwein or Cauchy steps, until either a candidate active set is identified or no reasonable progress toward the solution is made;
- a *minimization phase*, which reduces the objective function in the working set defined by the identification phase, by applying either the SDC or the SDA method recently proposed for unconstrained quadratic programming [3, 1].

Attention is devoted to the formulation of the reduced problem in the minimization phase, by taking into account information on the spectral properties of the reduced Hessian. The algorithmic framework also allows to exploit the effectiveness of SDA and SDC, as well

as their regularizing properties [2], in a constrained optimization setting. The results of numerical experiments carried out on several SLBQP problems show the effectiveness of the proposed approach.

References

[1] De Asmundis, R., di Serafino, D., Hager, W. W., Toraldo G., and Zhang, H. 2014 *An efficient gradient method using the Yuan steplength*. Comput. Optim. Appl. 59, 541–563.

[2] De Asmundis, R., di Serafino, D., and Landi, G. 2016 *On the regularizing behavior of the SDA and SDC gradient methods in the solution of linear ill-posed problems*. J. Comput. Appl. Math. 302, 81–93.

[3] De Asmundis, R., di Serafino, D., Riccio, F., and Toraldo, G. 2013 *On spectral properties of steepest descent methods*. IMA J. Numer. Anal. 33, 1416–1435.

[4] Meyer, R. R. 1984 *Multipoint methods for separable nonlinear networks*. Math. Programming Study 22, 185–205.

[5] Moré, J. J. and Toraldo, G. 1991 *On the solution of large quadratic programming problems with bound constraints*. SIAM J. Optim. 1, 93–113.

[6] Pardalos, P. M. and Rosen, J. B. (Eds.) 1987 *Constrained global optimization: algorithms and applications*. Lecture Notes in Computer Science, vol. 268, Springer.

[7] Vapnik,V. 1982 *Estimation of dependences based on empirical data*, Springer-Verlag.

Global/Local Hybridization of the Multi-Objective Particle Swarm Optimization with Derivative-Free Multi-Objective Local Search

Riccardo Pellegrini
Roma Tre University, Department of Mechanical and Industrial Engineering
Via Vito Volterra, 62 - Rome, Italy
riccardo.pellegrini@uniroma3.it

Umberto Iemma
Roma Tre University, Department of Mechanical and Industrial Engineering
Via Vito Volterra, 62 - Rome, Italy
umberto.iemma@uniroma3.it

Andrea Serani
CNR-INSEAN, Natl. Research Council-Marine Technology Research Institute
Via di Vallerano, 139 - Rome, Italy
andrea.serani@insean.cnr.it

Emilio F. Campana
CNR-INSEAN, Natl. Research Council-Marine Technology Research Institute
Via di Vallerano, 139 - Rome, Italy
emiliofortunato.campana@insean.cnr.it

Matteo Diez
CNR-INSEAN, Natl. Research Council-Marine Technology Research Institute
Via di Vallerano, 139 - Rome, Italy
matteo.diez@insean.cnr.it

Giampaolo Liuzzi
CNR-IASI, Natl. Research Council-Institute for Systems Analysis and Computer Science
Via dei Taurini, 19 - Rome, Italy
giampaolo.liuzzi@iasi.cnr.it

Francesco Rinaldi
University of Padua, Department of Mathematics
Via Trieste, 63 - Padua, Italy
rinaldi@math.unipd.it

Stefano Lucidi
Sapienza University, Department of Computer, Control, and Management Engineering "A. Ruberti"
Via Ariosto, 25 - Rome, Italy

lucidi@dis.uniroma1.it

Simulation Based Design Optimization (SBDO) supports the design of complex engineering systems. The process consists in the application of several numerical simulations with the aim of exploring and assessing the design opportunities among all the feasible design solutions. The multi-objective optimization algorithm manages the search of the best compromise between all the design objectives (such as the resistance and seakeeping of a ship or the drag and weight of an airplane), generally provided in terms of Pareto fronts.
The objective functions may be noisy and/or often their derivatives are not directly provided by the simulation tools. Therefore, derivative-free optimization algorithms are used as a viable option for the SBDO process. Local or global optimization algorithms are preferred, whether a fine search region is or is not known a priori. The first class of algorithms explores accurately a limited domain region, whereas the second explores efficiently the entire design space, providing approximate solutions to the decision problem.
In order to combine the accuracy of local algorithms with the exploration capability of global methods for multi-objective problems, a multi-objective deterministic particle swarm optimization (MODPSO) [4, 5] is combined with a derivative-free multi-objective (DFMO) [3] local optimization algorithm.
MODPSO is a multi-objective extension of the single-objective deterministic PSO [1, 6]. The global attractor of each swarm particle is the closest point of the global Pareto front. The personal attractor is selected using two different implementations, namely MODPSO1 and MODPSO3 (see, [4, 5]): MODPSO1 uses the closest point of the personal Pareto front; MODPSO3 uses the position associated with the personal minimum of an aggregated objective function. The global and personal attractor distances are computed in the variables domain.
DFMO is a derivative-free algorithm for constrained (possibly) non-smooth multi-objective problems. It is a so-called a "posteriori" method in the sense that it is able to approximate the entire Pareto front by producing in output a set of non-dominated points. More in particular, at every iteration, the algorithm produces (or updates) a set of non-dominated points (rather than a single point, as it is common in the single-objective case). As the iteration count grows, these sets of points tend to the real Pareto front of the problem. Other relevant features of DFMO are: i) a linesearch approach that takes into account the presence of multiple objectives; ii) an exact penalty approach for dealing with the nonlinear constraints.
At each iteration, for each point in the current set of non-dominated points, DFMO starts a linesearch along a suitably generated direction. If such a direction is able to guarantee "sufficient" decrease, then a "sufficiently" large movement along the direction is performed. This allows to (possibly) improve the current set of non-dominated points.
A non trivial issue about combining MODPSO and DFMO is to define when and where from the local search should starts. Herein, the local search associated to a specific particle starts when the particle speed decreases under a threshold value β.
The local search starts either from the current position of the particle or from the global attractor associated with the particle. The hybridization of MODPSO with DFMO is shown in the block diagram below (see Fig. 1), where N_p is the number of particles of MODPSO and $\mathbf{x}_i$ is the starting point for DFMO. The resulting global/local hybrid implementations (see Tab. 1) are tested using 45 analytical problems, with a number of variables ranging from 1 to 30 and a number of objectives ranging from 2 to 3. The per-

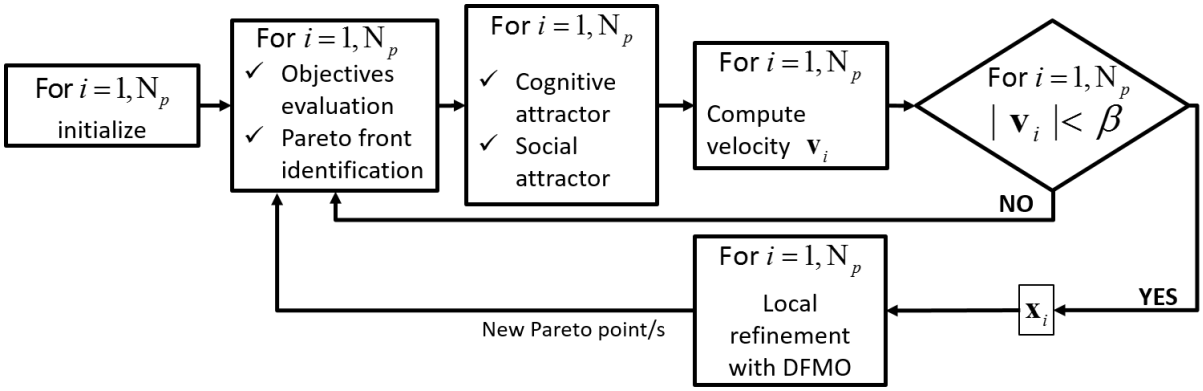


Figure 1: Hybridization scheme of MODPSO with DFMO

formances of the algorithms are assessed considering four metrics: Generational Distance (GD), Inverted Generational Distance (IDG) [7], their combination Generational Merit Factor (GMF) [4], and a normalized version of Hypervolume (NHV) [8, 2]. Figure 2 shows, on average, the performances of combined hybrid and separate global and local algorithms in terms of GD, IGD, GMF, and NHV. Lower values of GD, IGD, and GMF correspond to better performances, conversely higher values of NHV correspond to better performing algorithms. The hybrid algorithms overperform the separate global and local methods, starting form medium/high budgets of function evaluations. Figure 3 shows three examples of approximated Pareto fronts provided by DFMO, MODPSO3, and HMODPSO3-G. In conclusion, the hybridization of MODPSO with DFMO has

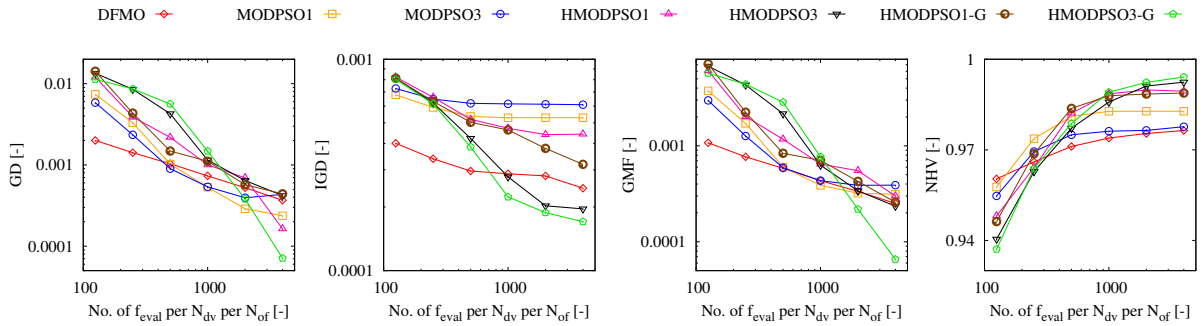


Figure 2: Average (over 45 analytical test problems) GD, IGD, GMF, and NHV for the best implementation of combined hybrid and separate global and local algorithms

been investigated, using two criteria for the activation of the local search. 45 analytical test problems and four performance metrics have been used in order to assess the algorithm performances. The hybrid algorithms have shown promising improvements for medium/high budgets of functions evaluations. Future work includes the investigation of additional criteria for activating the local search, based on the quality of the approximated Pareto front.

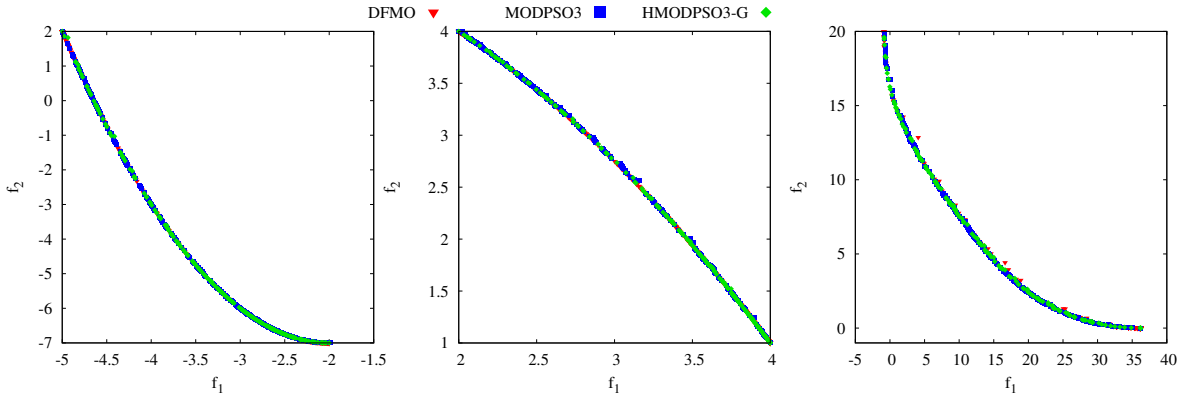


Figure 3: Examples of Pareto fronts, with comparison between combined hybrid and separate global and local algorithms

Algorithm	**MODPSO global attractor**	**MODPSO personal attractor**	**DFMO starting point**
HMODPSO1	Closest point of the global Pareto front	Closest point of the personal Pareto front	Particle position
HMODPSO3	Closest point of the global Pareto front	Personal minimum of an aggregated objective function	Particle position
HMODPSO1-G	Closest point of the global Pareto front	Closest point of the personal Pareto front	Global attractor
HMODPSO3-G	Closest point of the global Pareto front	Personal minimum of an aggregated objective function	Global attractor

Table 1: Hybrid algorithm nomenclature

References

[1] Campana, E. F., Liuzzi G., Lucidi S., Peri D., Piccialli V., and Pinto A. *New global optimization methods for ship design problems*, Optimization and Engineering, 4, 2009, 533–555.

[2] Fonseca C.M. , Paquete L., and Lòpez-Ibánez M. *An Improved Dimension-Sweep Algorithm for the Hypervolume indicator*, Proceedings of the 2006 IEEE International Conference on Evolutionary Computation (CEC'06), 1157–1163, Vancouver, BC, Canada, 16–21 July 2006.

[3] Liuzzi G., Lucidi S., and Rinaldi F. *A derivative-free approach to constrained multi-objective nonsmooth optimization*. Submitted for pubblication on SIAM journal on Optimization.

[4] Pellegrini, R., E. F. Campana, M. Diez, A. Serani, F. Rinaldi, G. Fasano, U. Iemma, G. Liuzzi, S. Lucidi, and F. Stern. *Application of derivative-free multi-objective algorithms to reliability-based robust design optimization of a high-speed catamaran*

in real ocean environment, Proceedings of the 4th International Conference on Engineering Optimization (EngOpt 2014), Lisbon, Portugal, 8–11 September 2014.

[5] Pellegrini R., Serani A., Diez M., Iemma U., and Campana E. F. *Multi-objective extensions of the deterministic particle swarm algorithm for RBRDO in ship design: a parametric study*. Proceedings of the 17th Numerical Towing Tank Symposium (NuTTS 2014), Marstrand, Sweden, 28–30 September 2014.

[6] Serani A., Diez M., Leotardi C., Peri D., Fasano G., Iemma U., and Campana E.F. *On the use of synchronous and asynchronous single-objective deterministic particle swarm optimization in ship design problems*, Proceedings of the 1st International Conference on Engineering and Applied Sciences Optimization (OPT-i 2014), Kos Island, Greece, June 2014.

[7] Van Veldhuizen, D.A. and Lamont, G.B. *Evolutionary computation and convergence to a Pareto front*, Late breaking papers at the genetic programming 1998 conference, Stanford University, California, 1998, 221–228.

[8] Zitzler, E. and Thiele, L. *Multiobjective optimization using evolutionary algorithms — A comparative case study*, Proceedings of 5th International Conference on Parallel Problem Solving from Nature (PPSN V), 292–301, Amsterdam, The Netherlands, 27–30 September 1998.

Regularizing Trust-region approaches for ill-posed nonlinear least squares problems

Stefania Bellavia
Università degli Studi di Firenze
Dipartimento di Ingegneria Industriale, viale G.B. Morgagni 40, 50134 Firenze, Italia
stefania.bellavia@unifi.it

Benedetta Morini
Università degli Studi di Firenze
Dipartimento di Ingegneria Industriale, viale G.B. Morgagni 40, 50134 Firenze, Italia
benedetta.morini@unifi.it

Elisa Riccietti
Università degli Studi di Firenze
Dipartimento di Matematica e Informatica, viale G.B. Morgagni 67a, 50134 Firenze, Italia
elisa.riccietti@unifi.it

In this talk we will address the numerical solution of ill-posed, potentially rank-deficient, nonlinear systems and nonlinear least-squares. We will analyse algorithms belonging to a trust-region framework. The noise-free case as well as the realistic situation where noisy data are given will be considered and conditions under which these methods can be seen as regularizing methods for ill-posed problems will be given. The methods rely on a trust region radius choice ensuring regularizing properties and giving rise to a procedure that has the potential to approximate a solution of the unperturbed problem. In the noise-free case the trust-region radius plays the double role of providing global convergence and handling the ill-posedness of the problems.
Effectiveness of the method will be illustrated on nonlinear systems arising from the discretization of Fredholm equations of the first kind and on data-fitting problems arising in geophysical applications.

Isogeometric Methods: theoretical and computational aspects - Part I

PROPOSERS

Giancarlo Sangalli
Dipartimento di Matematica, Università di Pavia
Via Ferrata 1, 27100 - Pavia, Italy
giancarlo.sangalli@unipv.it

Lorenzo Tamellini
Istituto di Matematica Applicata e Tecnologie Informatiche (IMATI) - CNR
Via Ferrata 1, 27100 - Pavia, Italy
tamellini@imati.cnr.it

SPEAKERS

Thomas Takacs
Inst. for Applied Geometry, J. Kepler University Linz
thomas.takacs@jku.at

Andrea Bressan
Inst. for Applied Geometry, J. Kepler University Linz
Andrea.Bressan@jku.at

Hendrik Speleers
Dip. Matematica, Uni. di Roma "Tor Vergata"
speleers@mat.uniroma2.it

Carlotta Giannelli
Dip. Matematica e Informatica, Uni. Firenze
carlotta.giannelli@unifi.it

Andrea Bartezzaghi
MATHICSE-CMCS, EPFL
andrea.bartezzaghi@epfl.ch

Stefano Serra Capizzano
Dip. Matem. e Fisica, Uni. Insubria
stefano.serrac@uninsubria.it

Isogeometric Analysis (IGA) has been introduced to bridge the gap between Computer Aided Design and PDE-based engineering analysis. A well-established mathematical theory based on using Non-Uniform Rational B-Splines (NURBS) instead of Finite Element basis functions has thus been developed, and nowadays IGA can be successfully applied to solid, fluid, and multiphysics problems, and even outperform the standard Finite Element analysis in certain circumstances.
Yet, significant challenges remain open, such as the application of the method to domains described by trimming (boolean) operations, the development of local refinement technolo-

gies and of algorithms capable of reducing assembly costs for high-order approximations, as well as the analysis of collocation schemes.
The purpose of this symposium is to bring together scientists and practitioners active in the field of IGA with the aim of contributing to further advance its state of the art.

Approximation with C1 smooth isogeometric functions over multi-patch domains

Thomas Takacs
Johannes Kepler Unversity Linz
Altenberger Str. 69, 4040 - Linz, Austria
thomas.takacs@jku.at

Given a physical domain $\Omega \subset \mathbb{R}^2$, we consider a geometry parametrization of Ω that is composed of multiple B-spline patches forming a regular partition. On this multi-patch representation we define a standard isogeometric function space. We discuss the approximation error properties of the C^1-smooth subspace of such an isogeometric space. We show that if the space is an *analysis-suitable* C^1 *multi-patch isogeometric space* the convergence rate is optimal under h-refinement. If the parametrization is not analysis-suitable, optimal convergence is prevented. Note that analysis-suitable geometries cover but are not limited to piecewise bilinear parametrizations. The results presented here are based on [1].

References

[1] A. Collin, G. Sangalli and T. Takacs. Analysis-suitable G^1 multi-patch parametrizations for C^1 isogeometric spaces. *Computer Aided Geometric Design*, in press, 2016.

Quasi-interpolants for non-tensor-product spline spaces

Andrea Bressan
IMATI CNR Pavia via Ferrata, 1 27100 - Pavia Italy
andrea.bressan.ab@gmail.com

Tom Lyche
University of Oslo
Moltke Moes vei, 35 0851 - Oslo Norway
tom@math.uio.no

Splines spaces that allow for different detail level in different regions of the domain have been developed in the last two decades. In order to study the approximation properties of those spaces it is convenient to use quasi-interpolants: local coefficient-based linear operators on the spline space [1]. This talk will present the construction of quasi-interpolants for LR-spline and the resulting approximation estimates. The construction is based on [2].

References

[1] Lyche, T. and Schumaker, L. L. 1975 *Local spline approximation methods.* J. Approximation Theory. 15(4), 294–325.

[2] Bressan, A. 2013 *Some properties of LR-splines* . Comput. Aided Geom. Design. 30(8), 294–325

Quasi-interpolants and local approximation estimates for hierarchical spline spaces

Hendrik Speleers
Università degli Studi di Roma "Tor Vergata"
Via della Ricerca Scientifica - 00133 Roma, Italy
speleers@mat.uniroma2.it

The term *quasi-interpolation* denotes a general approach to construct, with a low computational cost, efficient approximants to a given set of data or a given function. A quasi-interpolant is usually obtained as a linear combination of the elements of a suitable set of functions that form a convex partition of unity and possess a small local support. These properties ensure both numerical stability and local control of the constructed approximant. Quasi-interpolants in polynomial spline spaces are a common and powerful approximation tool.

In this talk we focus on quasi-interpolants in hierarchical spline spaces. Such spline spaces provide a flexible framework for local refinement coupled with a remarkable intrinsic simplicity. They are defined in terms of a hierarchy of locally refined meshes, reflecting different levels of refinement. The so-called *truncated hierarchical B-spline (THB-spline) basis* is an interesting basis for the hierarchical spline space with an enhanced set of properties compared to the classical hierarchical B-spline basis [1, 4]. The THB-spline basis forms a convex partition of unity, its elements are more locally supported than those of the classical hierarchical basis, and it is strongly stable with respect to the supremum norm [2, 3].

We discuss a general approach to construct local quasi-interpolants in hierarchical spline spaces expressed in terms of the THB-spline basis [5, 6]. The main ingredient is the property of *preservation of coefficients* of the THB-spline representation. Thanks to this property, the construction of the hierarchical quasi-interpolant is basically effortless. It is sufficient to consider a local quasi-interpolant in each space associated with a particular level in the hierarchy, which will be referred to as a one-level quasi-interpolant. Then, the coefficients of the proposed hierarchical quasi-interpolant are nothing else than a proper subset of the coefficients of the one-level quasi-interpolants. No additional manipulations are required. Important properties – like polynomial reproduction – of the one-level quasi-interpolants are preserved in the hierarchical construction. We also discuss the local approximation order of the hierarchical quasi-interpolants in different norms. Finally, we confirm the effectiveness of the approach with some numerical examples.

Both the construction and the approximation theory of hierarchical quasi-interpolants are detailed in terms of hierarchies of truncated tensor-product polynomial B-splines, due to their relevant interest. Nevertheless, the approach is completely general and can be easily rephrased towards a broad framework of sets of basis functions (see [3, 5]).

References

[1] Forsey, D.R., Bartels, R.H. (1988) *Hierarchical B-spline refinement.* ACM SIGGRAPH Computer Graphics 22, 205–212.

[2] Giannelli, C., Jüttler, B., Speleers, H. (2012) *THB-splines: The truncated basis for hierarchical splines*. Computer Aided Geometric Design 29, 485–498.

[3] Giannelli, C., Jüttler, B., Speleers, H. (2014) *Strongly stable bases for adaptively refined multilevel spline spaces*. Advances in Computational Mathematics 40, 459–490.

[4] Kraft, R. (1997) *Adaptive and linearly independent multilevel B-splines*. In: Le Méhauté, A., Rabut, C., Schumaker, L.L. (eds.), Surface Fitting and Multiresolution Methods, pp. 209–218. Vanderbilt University Press, Nashville.

[5] Speleers, H., Manni, C. (2016) *Effortless quasi-interpolation in hierarchical spaces*. Numerische Mathematik 132, 155–184.

[6] Speleers, H. (2016) *Hierarchical spline spaces: Quasi-interpolants and local approximation estimates*. Preprint.

Adaptivity with hierarchical splines: optimality

Carlotta Giannelli
Università degli Studi di Firenze
viale Morgagni, 67/a 50134 - Firenze Italy
carlotta.giannelli@unifi.it

Annalisa Buffa
Istituto di Matematica Applicata e Tecnologie Informatiche del CNR
via Ferrata, 1 27100 - Pavia Italy
annalisa@imati.cnr.it

We consider an adaptive isogeometric method (AIGM) for solving elliptic second-order partial differential equations with truncated hierarchical B-splines of arbitrary degree and different order of continuity in any space dimension. Preliminary results on approximation, efficient and reliable error estimates and convergence of the adaptive procedure, have been recently presented [1]. The complexity estimate of the mesh refinement procedure proposed in [1] was also addressed [2]. By starting from an inital configuration, this estimate guarantees a certain bound for the ratio between the number of refined elements in the final mesh and the number of all marked elements along the sequence of successive refinements.
In order to derive a local upper bound of the error, we extend the analysis of residual-type error estimator for the considered AIGM. This is achieved by suitably combining a class of stable quasi-interpolation operators onto the space of splines on tensor-product meshes with the hierarchical construction. The talk will present the theoretical framework to link the adaptive method with optimal meshes to related approximation classes by proving the quasi-optimal cardinality of the AIGM.

References

[1] Buffa, A. and Giannelli, C. 2016 *Adaptive isogeometric methods with hierarchical splines: Error estimator and convergence*. Math. Models Methods Appl. Sci. 26, 1–25.

[2] Buffa, A., Giannelli, C., Morgenstern, P. and Peterseim, D. 2016 *Complexity of hierarchical refinement for a class of admissible mesh configurations*. Comput. Aided Geom. Design, to appear.

Isogeometric Analysis for the Modeling of Red Blood Cells

Andrea Bartezzaghi
CMCS–MATHICSE–SB, École Polytechnique Fédérale de Lausanne
Av. Piccard, Station 8, CH-1015, Lausanne, Switzerland
andrea.bartezzaghi@epfl.ch

Luca Dedè
CMCS–MATHICSE–SB, École Polytechnique Fédérale de Lausanne
Av. Piccard, Station 8, CH-1015, Lausanne, Switzerland
luca.dede@epfl.ch

Alfio Quarteroni
CMCS–MATHICSE–SB, École Polytechnique Fédérale de Lausanne
Av. Piccard, Station 8, CH-1015, Lausanne, Switzerland
alfio.quarteroni@epfl.ch

In this talk, we consider the mathematical modeling of red blood cells (RBCs), which together with plasma, white blood cells, and platelets, constitute the blood. RBCs are the principal factor of blood rheology since they outnumber the other cells and platelets, especially in small vessels (the capillaries). In this work, we model the RBC lipid bi-layer biomembrane as a surface in the 3D space, whose evolution in time is governed by a geometric Partial Differential Equation (PDE) deriving from the minimization of the bending energy under area and volume constraints, also called Canham–Helfrich energy [5].
The geometric PDEs modeling the shape of RBCs involve high order surface differential operators and result in a time dependent nonlinear problem [3]. From this point of view, we consider the spatial approximation of the geometric PDEs modeling the RBC by means of NURBS-based Isogeometric Analysis (IGA) [4] in the framework of the Galerkin method. The RBCs' membranes are represented by smooth single-patch NURBS surfaces. The use of NURBS with high order of continuity of the basis functions leads to efficient treatment of the high order differential operators [2]; moreover, it allows for accurate evaluations of the geometrical quantities involved in the geometric PDEs [1]; we satisfy the area and volume constraints of the RBC by means of Lagrange multipliers. For the time discretization of the PDEs we propose Backward Differentiation Formulas with extrapolation of the geometric quantities and semi-implicit treatment of the area and volume preservation constraints. We show and discuss numerical results obtained in approximating geometric PDEs with IGA, highlighting that, with a limited amount of degrees of freedom, it is yielding very accurate geometric representation of RBCs.
Finally, we present and discuss numerical simulations for RBC modeling coupled with plasma flow. We propose a non-boundary-fitted discretization of the fluid domain with respect to the shape of the RBC. The presence of the biomembrane is accounted weakly in the fluid formulation, while RBCs are treated as geometric PDEs. We present and discuss some results for this numerical coupling.

References

[1] Bartezzaghi, A., Dedè, L. and Quarteroni, A. 2016 *Isogeometric Analysis of Geometric Partial Differential Equations*. MATHICSE report 11.2016, *submitted to Computer Methods in Applied Mechanics and Engineering*.

[2] Bartezzaghi, A., Dedè, L. and Quarteroni, A. 2015 *Isogeometric Analysis of high order Partial Differential Equations on surfaces*. Computer Methods in Applied Mechanics and Engineering 295, 446–469.

[3] Bonito, A., Nochetto, R. H. and Pauletti, M. S. 2011 *Dynamics of biomembranes: effect of the bulk fluid*. Mathematical Modeling of Natural Phenomena 6, 25–43.

[4] Cottrell, J. A., Hughes, T. J. R. and Bazilevs, Y. 2009 *Isogeometric Analysis: toward integration of CAD and FEA*. Wiley.

[5] Canham, P. B. 1970 *The minimum energy of bending as a possible explanation of the biconcave shape of the human red blood cell*. Journal of Theoretical Biology 26, 61–81.

GLT analysis, symbol, IgA and FEM approximations of partial differential equations

Stefano Serra Capizzano
Università degli Studi dell'Insubria - Sede di Como- DISAT
via Valleggio, 11 22100 - Como Italy
Uppsala University - Information Technology Department
Box 337, SE-751 05 - Uppsala, Sweden
stefano.serrac@uninsubria.it, stefano.serra@it.uu.se

Recently, the class of Generalized Locally Toeplitz (GLT) sequences has been introduced [18, 19] as a generalization both of classical Toeplitz sequences and of variable coefficient differential operators and, for every sequence of the class, it has been demonstrated that it is possible to give a rigorous description of the asymptotic spectrum [3, 22] in terms of a function (the symbol) that can be easily identified; see also [21].
This generalizes the notion of a symbol for differential operators (discrete and continuous) or for Toeplitz sequences for which it is identified through the Fourier coefficients and is related to the classical Fourier Analysis.
The GLT class has nice algebraic properties and indeed it has been proven that it is stable under linear combinations, products, and inversion when the sequence which is inverted shows a sparsely vanishing symbol (sparsely vanishing symbol = a symbol which vanishes at most in a set of zero Lebesgue measure). Furthermore, the GLT class virtually includes any approximation of partial differential equations (PDEs) by local methods (Finite Difference, Finite Element, Isogeometric Analysis [4, 5, 20] etc) and, based on this, we demonstrate that our results on GLT sequences can be used in a PDE setting in various directions:

1. as a generalized Fourier Analysis for the design and for the study of preconditioned iterative and semi-iterative methods, when dealing with variable coefficients, non rectangular domains, non uniform gridding or triangulations,

2. for a multigrid analysis of convergence and for providing spectral information on large preconditioned systems in the variable coefficient case,

3. in order to provide a tool for the stability analysis of PDE numerical schemes (e.g. a necessary von Neumann criterium for variable coefficient systems of PDEs is obtained, uniformly with respect to the boundary conditions), etc.

We will discuss specifically problems 1) and 2), with special attention to the IgA setting, and other possible directions in which the GLT analysis can be conveniently employed; see below for a recent bibliography on the subject.

The present work includes collaborations with Donatelli, Dorostkar, Garoni, Golinskii, Hughes, Kuijlaars, Manni, Mazza, Molteni, Neytcheva, Pelosi, Pennati, Ratnani, Reali,Semplice, Sesana, Speleers.

References

[1] A. Aricò, M. Donatelli, S. Serra-Capizzano. V-cycle optimal convergence for certain (multilevel) structured linear systems. *SIAM J. Matrix Anal. Appl.* **26** (2004), 186–214.

[2] B. Beckermann, S. Serra-Capizzano. On the asymptotic spectrum of Finite Element matrix sequences. *SIAM J. Numer. Anal.* **45** (2007), 746–769.

[3] A. Böttcher, B. Silbermann. *Introduction to Large Truncated Toeplitz Matrices.* Springer-Verlag, New York (1999).

[4] P.G. Ciarlet. *The Finite Element Method for Elliptic Problems.* SIAM (2002).

[5] J.A. Cottrell, T.J.R. Hughes, Y. Bazilevs. *Isogeometric Analysis: Toward Integration of CAD and FEA.* John Wiley & Sons, New York (2009).

[6] M. Donatelli, C. Garoni, C. Manni, S. Serra-Capizzano, H. Speleers. Robust and optimal multi-iterative techniques for IgA Galerkin linear systems. *Comput. Methods Appl. Mech. Engrg.* **284** (2015), 230–264.

[7] M. Donatelli, C. Garoni, C. Manni, S. Serra-Capizzano, H. Speleers. Robust and optimal multi-iterative techniques for IgA collocation linear systems. *Comput. Methods Appl. Mech. Engrg.* **284** (2015), 1120–1146.

[8] M. Donatelli, C. Garoni, C. Manni, S. Serra-Capizzano, H. Speleers. Spectral analysis and spectral symbol of matrices in isogeometric collocation methods. *Math. Comp.* **85** (2016); S0025-5718-2015-03027-0.

[9] M. Donatelli, M. Mazza, S. Serra-Capizzano. Spectral analysis and preconditioning for variable coefficient fractional derivative operators. it J. Comput. Phys. **307** (2016), 262–279. Tech. Report 2015-002, Div. Scientific Computing, Uppsala University (2015).

[10] A. Dorostkar, M. Neytcheva, S. Serra-Capizzano. Spectral analysis of coupled PDEs and of their Schur complements via the notion of Generalized Locally Toeplitz sequences. *Comput. Methods Appl. Mech. Engrg.* , under revision. Tech. Report 2015-008, Div. Scientific Computing, Uppsala University (2015).

[11] C. Garoni, C. Manni, F. Pelosi, S. Serra-Capizzano, H. Speleers. On the spectrum of stiffness matrices arising from isogeometric analysis. *Numer. Math.* **127** (2014), 751–799.

[12] C. Garoni, C.Manni, S. Serra-Capizzano, D. Sesana, H. Speleers. Spectral analysis and spectral symbol of matrices in isogeometric Galerkin methods. *Math. Comp.* , in press. Tech. Report 2015-005, Div. Scientific Computing, Uppsala University (2015).

[13] C. Garoni, S. Serra-Capizzano, D. Sesana. Spectral Analysis and Spectral Symbol of d-variate Q_p Lagrangian FEM Stiffness Matrices. *SIAM J. Matrix Anal. Appl.* **36-3** (2015), 1100–1128

[14] C. Garoni, S. Serra-Capizzano, P. Vassalos. A general tool for determining the asymptotic spectral distribution of Hermitian matrix-sequences. *Oper. Matrices* **9-3** (2015), 549–561.

[15] L. Golinskii, S. Serra-Capizzano. The asymptotic properties of the spectrum of nonsymmetrically perturbed Jacobi matrix sequences. *J. Approx. Theory* **144** (2007), 84–102.

[16] S. Serra-Capizzano. Matrix algebra preconditioners for multilevel Toeplitz matrices are not superlinear, *Linear Algebra Appl.* **343–344** (2002), 303–319.

[17] S. Serra-Capizzano. Convergence analysis of two-grid methods for elliptic Toeplitz and PDEs matrix-sequences. *Numer. Math.* **92** (2002), 433–465.

[18] S. Serra-Capizzano. Generalized Locally Toeplitz sequences: spectral analysis and applications to discretized partial differential equations. *Linear Algebra Appl.* **366** (2003), 371–402.

[19] S. Serra-Capizzano. The GLT class as a generalized Fourier Analysis and applications. *Linear Algebra Appl.* **419** (2006), 180–233.

[20] J.C. Strikwerda. *Finite Difference Schemes and Partial Differential Equations.* SIAM (2004).

[21] P. Tilli. Locally Toeplitz sequences: spectral properties and applications. *Linear Algebra Appl.* **278** (1998), 91–120.

[22] E.E. Tyrtyshnikov. A unifying approach to some old and new theorems on distribution and clustering. *Linear Algebra Appl.* **232** (1996) 1–43.

Isogeometric Methods: theoretical and computational aspects - Part II

PROPOSERS

Giancarlo Sangalli
Dipartimento di Matematica, Università di Pavia
Via Ferrata 1, 27100 - Pavia, Italy
giancarlo.sangalli@unipv.it

Lorenzo Tamellini
Istituto di Matematica Applicata e Tecnologie Informatiche (IMATI) - CNR
Via Ferrata 1, 27100 - Pavia, Italy
tamellini@imati.cnr.it

SPEAKERS

Mattia Tani
Dip. Matematica, Università di Pavia
mattia.tani@unipv.it

Lorenzo Tamellini
IMATI - CNR
tamellini@imati.cnr.it

Francesco Calabrò
Dip. Ing. Elettrica e Informazione, Università di Cassino
calabro@unicas.it

Luca Heltai
SISSA - Trieste
luca.heltai@sissa.it

Rafael Vázquez
IMATI - CNR
vazquez@imati.cnr.it

Massimiliano Martinelli
IMATI - CNR
martinelli@imati.cnr.it

Isogeometric Analysis (IGA) has been introduced to bridge the gap between Computer Aided Design and PDE-based engineering analysis. A well-established mathematical theory based on using Non-Uniform Rational B-Splines (NURBS) instead of Finite Element basis functions has thus been developed, and nowadays IGA can be successfully applied to solid, fluid, and multiphysics problems, and even outperform the standard Finite Element analysis in certain circumstances.
Yet, significant challenges remain open, such as the application of the method to domains described by trimming (boolean) operations, the development of local refinement technolo-

gies and of algorithms capable of reducing assembly costs for high-order approximations, as well as the analysis of collocation schemes.
The purpose of this symposium is to bring together scientists and practitioners active in the field of IGA with the aim of contributing to further advance its state of the art.

Isogeometric preconditioners based on fast solvers for the Sylvester equation

Mattia Tani
Università di Pavia
via A. Ferrata, 5 27100 - Pavia Italy
mattia.tani@unipv.it

Giancarlo Sangalli
Università di Pavia
via A. Ferrata, 5 27100 - Pavia Italy
giancarlo.sangalli@unipv.it

We address the problem of numerically solving linear systems that arise in Isogeometric Analysis (IGA). It is known that many standard methods, when applied to IGA systems, have a computational cost which significantly increase with the degree p of the splines employed as basis functions. This fact contributes in making high degree splines prohibitive for real world applications. As a consequence, a number of recent papers have attempted to reduce the dependence of computational cost from p.
Let $\mathcal{K}$ be the stiffness matrix for the Poisson problem on an arbitrary physical domain. A simple but crucial observation is that $\mathcal{K}$ can be preconditioned by the stiffness matrix for the unit hypercube, which has the form

$$\mathcal{P} = \sum_{i=1}^{d} M_1 \otimes \ldots \otimes M_{i-1} \otimes K_i \otimes M_{i+1} \otimes \ldots \otimes M_d,$$

where M_i and K_i, $i = 1, \ldots, d$, represent one-dimensional mass and stiffness matrices, and d is the problem dimension.
Our approach is based on the fact that the application of $\mathcal{P}^{-1}$ is equivalent to the solution of a tensor equation. For example, when $d = 2$ the linear system $\mathcal{P}s = r$ is equivalent to the solution of the matrix equation

$$M_2 S K_1 + K_2 S M_1 = R$$

where S and R are matrices obtained by a proper reshape of vectors s and r.
The literature on the numerical solution of such problems is vast, and we select among the available methods the ones which seem the most suited for the particular features of IGA problems. Application to 2D and 3D problems is shown, and robustness with respect to the problems parameters (such as the spline degree) is discussed. We also discuss how the geometry of the PDE domain affects the spectral properties of $\mathcal{P}^{-1}\mathcal{K}$, and propose simple strategies to partially include information on the geometry in the preconditioner. Finally, we show how to combine the considered preconditioners with a domain decomposition appraoch in order to solve multipatch problems with conforming discretization.

A sparse-grid version of IGA methods

Lorenzo Tamellini
IMATI-CNR
via Ferrata, 1 27100 - Pavia Italy
tamellini@imati.cnr.it

Giancarlo Sangalli
Università di Pavia
via Ferrata, 5 27100 - Pavia Italy
giancarlo.sangalli@unipv.it

Sparse grids have been proposed in the early 90's in the context of finite differences (FD) / finite elements (FE) methods to reduce the "curse of dimensionality effect", i.e., the fact that the number of degrees of freedom (DoF) of the approximation grows exponentially in the number of dimensions of the problem. Roughly speaking, the sparse-grid construction consists in recasting the construction of conventional FE/FD methods in a hierarchical fashion and suitably discarding the components which carry the least amount of information. Under suitable regularity assumptions (slightly more demanding than the usual Sobolev spaces) sparse grids are then able to deliver approximations with essentially the same accuracy of conventional FE/FD methods (i.e., up to a logarithmic factor appearing in the error estimates), using however a much lower number of DoF. Furthermore, the sparse-grid solution can be computed as a linear combination of standard FE/FD solutions on relatively coarse grids (the so-called "combination technique"): this implies that sparse grids can be implemented quite straightforwardly reusing existing solvers and leads to a very natural parallelization of the computation. In this talk we detail the application of the sparse-grid technology to the h-refined version of the classical IGA method and show some numerical tests that will highlight how sparse IGA performs compared to the classical "full tensor" counterpart.

Efficient Quadrature for High Degree Isogeometric Analysis

Francesco Calabrò
Università degli Studi di Cassino e del Lazio Meridionale
Via G. De Biasi 43 - 03043 Cassino (FR) Italy
calabro@unicas.it

Giancarlo Sangalli
Università degli Studi di Pavia
via Ferrata, 1 - 27100 Pavia Italy
giancarlo.sangalli@unipv.it

Mattia Tani
Università degli Studi di Pavia
via Ferrata, 1 - 27100 Pavia Italy
mattia.tani@unipv.it

We propose an algorithm for the formation of matrices of isogeometric Galerkin methods. The algorithm is based on a loop on the rows of the matrix and on the calculation of the row entries by weighted quadrature. The test function is incorporated in the integration weight while the trial function, the geometry parametrization and the PDEs coefficients form the integrand function. This approach is very effective in reducing the computational cost, while keeping the optimal order of approximation of the method. The analysis of the costs is confirmed by the numerical testing, where we show that surprisingly, for p large enough, the time required by the floating point operations is even less than the time spent in the unavoidable memory operations (allocation and memory write). Not only our algorithm allows a significant saving for low degrees spline, but also it paves the way to the use of high degree high order k-refinement in isogeometric analysis.

References

[1] Antolin, P. and Buffa, A. and Calabrò, F. and Martinelli, M. and Sangalli, G. 2015 *Efficient matrix computation for tensor-product isogeometric analysis: The use of sum factorization*, Computer Methods in Applied Mechanics and Engineering 285, 817–828.

[2] Calabrò, F. and Sangalli G. and Tani M. 2016, *Fast formation of isogeometric Galekin matrices by weighted quadrature*, arXiv:1605.01238.

[3] Hughes, T. J. R. and Reali, A. and Sangalli, G. 2010, *Efficient quadrature for NURBS-based isogeometric analysis*, Computer Methods in Applied Mechanics and Engineering 199, 301–313.

A natural framework for isogeometric fluid-structure-interaction: coupling BEM and Shell models

Luca Heltai
SISSA - International School for Advanced Studies, Trieste, Italy
luca.heltai@sissa.it

Josef Kiendl
Institute for Applied Mechanics, Technische Universität Braunschweig, Germany
j.kiendl@tu-braunschweig.de

Antonio DeSimone
SISSA - International School for Advanced Studies, Trieste, Italy
desimone@sissa.it

Alessandro Reali
Department of Civil Engineering and Architecture, University of Pavia, Italy
alereali@unipv.it

The interaction between thin structures and incompressible Newtonian fluids is ubiquitous both in nature and in industrial applications. We present an isogeometric formulation of such problems which exploits a boundary integral formulation of Stokes equations [1] to model the surrounding flow, and a non linear Kirchhoff-Love shell theory [2, 3] to model the elastic behaviour of the structure. We propose three different coupling strategies: a monolithic, fully implicit coupling, a staggered, elasticity driven coupling, and a novel semi-implicit coupling, where the effect of the surrounding flow is incorporated in the non-linear terms of the solid solver through its damping characteristics. The novel semi-implicit approach is then used to demonstrate the power and robustness of our method, which fits ideally in the isogeometric paradigm, by exploiting only the boundary representation (B-Rep) of the thin structure middle surface.

We are interested in studying the interaction between a thin deformable elastic body and an incompressible fluid. We consider a model problem where the inertial terms of the fluid are negligible when compared with both the fluid viscosity and the inertial terms of the solid. We assume that the deformable body occupies at time t the region $\Omega^{\mathrm{s}}(t) = \boldsymbol{x}(\Omega^{\mathrm{s}}_0) \subset \Re^3$ and that the rest of the space is entirely occupied by an incompressible fluid whose time dependent domain is $\Omega^{\mathrm{f}}(t) = \Re^3 \setminus \Omega^{\mathrm{s}}(t)$.

The fluid and solid domains are coupled through non-slip conditions and through balance equations across the boundary of the solid domain $\Gamma^{\mathrm{fsi}}(t) := \partial\Omega^{\mathrm{s}}(t)$.

We restrict our attention to problems for which $\Omega^{\mathrm{s}}(t)$ is a thin shell and we consider the Kirchhoff-Love shell theory, where the director, i.e., a vector normal to the middle surface, is assumed to remain normal to the middle surface in the deformed configuration (i.e., parallel to $\boldsymbol{g}_3$). With this assumption, the configuration of the shell is uniquely determined once we know the configuration of its middle surface $\Gamma(t)$, making this an

ideal candidate for a coupled FSI problem which requires only a surface description.
To summarise:

- the inertial terms of the fluid are negligible when compared with both the fluid viscosity and the inertial terms of the solid;
- the transversal dimension h of the solid is much smaller than all other directions, and can be neglected when considering the geometry of the problem;
- the coupling conditions between the solid and the fluid are applied *at the middle surface* $\Gamma(t)$ of the solid.

The fluid equations then reduce to Stokes equations on the domain $\Re^3 \setminus \Gamma(t)$, which are solved using an IGA Boundary Element Method technique. For a given prescribed velocity on $\Gamma(t)$, we can compute the force per unit area that the fluid exerts on the middle surface of the solid, by pulling the *jump* of the fluid normal stress on $\Gamma(t)$ back to the solid reference configuration.
We define the operator that performs this pull back $D\mathcal{N}_{\boldsymbol{u}}$, i.e., a *Dirichlet to Neumann map* such that:

$$\boldsymbol{f}^{\text{fsi}} = J D\mathcal{N}_{\boldsymbol{u}} \boldsymbol{v}_g. \tag{1}$$

Stresses in the solid are represented by the stress resultants $\boldsymbol{n}$ and $\boldsymbol{m}$, which are the normal forces and bending moments, respectively.
The final fluid-structure interaction system has the form

$$\int_{\Gamma_0} \left(\rho \ddot{\boldsymbol{u}} \cdot \delta \boldsymbol{u} - J \left(D\mathcal{N}_{\boldsymbol{u}} \dot{\boldsymbol{u}} \right) \delta \boldsymbol{u} \boldsymbol{n} : \delta \boldsymbol{\varepsilon} + \boldsymbol{m} : \delta \boldsymbol{\kappa} - \boldsymbol{b} \cdot \delta \boldsymbol{u} \right) \mathrm{d}A = 0, \qquad \forall \delta \boldsymbol{u} \in H^2(\Gamma_0) \tag{2}$$

Given the linearity of the problem in both $\ddot{\boldsymbol{u}}$ and $\dot{\boldsymbol{u}}$, a possible solution strategy is to introduce a time discretization $\mathcal{T} := \{t_0, t_1, \dots, t_N = T\}$ and write $\boldsymbol{u}_k := \boldsymbol{u}(t_k)$. At each time step k, we can approximate $\dot{\boldsymbol{u}}_k$ and $\ddot{\boldsymbol{u}}_k$ as a linear combination of the previous solution steps $\boldsymbol{u}_p$ with $p \leq k$, such that the problem reduces to a nonlinear system in $\boldsymbol{u}_k$ (here expressed in operator form, where $\mathcal{C}$ is the Dirchlet to Neumann map):

$$\mathcal{M} \ddot{\boldsymbol{u}}_k - \mathcal{C}(\boldsymbol{u}_k) \dot{\boldsymbol{u}}_k + \mathcal{P}(\boldsymbol{u}_k) - \mathcal{F}_k =: \mathcal{R}(\boldsymbol{u}_k) = 0 \qquad \text{in } V^*, \tag{3}$$

whose solution can be formally computed by a Newton iteration method, i.e., given a guess $\boldsymbol{u}_k^0 = \boldsymbol{u}_{k-1}$, we compute $\boldsymbol{u}_k^{m+1} = \boldsymbol{u}_k^m + \Delta \boldsymbol{u}_k^m$ where formally

$$\Delta \boldsymbol{u}_k^m = -(D_{\boldsymbol{u}} \mathcal{R}(\boldsymbol{u}_k^m))^{-1} \mathcal{R}(\boldsymbol{u}_k^m), \tag{4}$$

where $\mathcal{R}(\boldsymbol{u}_k^m)$ is the residual at step m, and the term $D_{\boldsymbol{u}} \mathcal{R}(\boldsymbol{u}_k^m)$ contains the Fréchet derivative of the residual w.r.t. $\boldsymbol{u}$, evaluated at $\boldsymbol{u}_k^m$, i.e.,

$$D_{\boldsymbol{u}} \mathcal{R}(\boldsymbol{u}_k^m) = c_0 \mathcal{M} - c_1 \mathcal{C}(\boldsymbol{u}_k^m) + D_{\boldsymbol{u}} \mathcal{C}(\boldsymbol{u}_k^m) \dot{\boldsymbol{u}}_k^m + D_{\boldsymbol{u}} \mathcal{P}(\boldsymbol{u}_k^m), \tag{5}$$

where c_0 and c_1 are the linear coefficients of the $\boldsymbol{u}_k$ term used to approximate $\ddot{\boldsymbol{u}}_k$ and $\dot{\boldsymbol{u}}_k$. The Fréchet derivative in equation (5) translates to the Jacobian of the residual in a finite dimensional setting. If computed directly using equation (5), such a Jacobian can be quite complex to approximate, and several simplifications can be proposed, leading to a Newton-Rapson iteration method in which the Jacobian of the residual is not exact, but only approximate.

Among these methods, the most commonly used are *segregated* methods, where the solution of the fluid system is done separately with respect to the solution of the solid system. These methods are equivalent to a variation of the following systems of equations

$$\mathcal{M}\ddot{\boldsymbol{u}}_k - \mathcal{C}(\boldsymbol{u}_{k-1})\dot{\boldsymbol{u}}_{k-1} + \mathcal{P}(\boldsymbol{u}_k \quad) - \mathcal{F}_k = 0 \qquad \text{in } V^* \tag{6}$$

$$\mathcal{M}\ddot{\boldsymbol{u}}_k - \mathcal{C}(\boldsymbol{u}_k \quad)\dot{\boldsymbol{u}}_k \quad + \mathcal{P}(\boldsymbol{u}_{k-1}) - \mathcal{F}_k = 0 \qquad \text{in } V^*, \tag{7}$$

either solid-dominated segregated FSI schemes or fluid-dominated segregated FSI schemes. The structure of the problem suggests naturally a semi-implicit solution scheme, in which the nonlinearity of the fluid structure interaction is removed from the system, by evaluating the fluid structure operator at the previous time step, but retaining the evaluation of the velocity field at the current time step, i.e., solving

$$\mathcal{M}\ddot{\boldsymbol{u}}_k - \mathcal{C}(\boldsymbol{u}_{k-1})\dot{\boldsymbol{u}}_k + \mathcal{P}(\boldsymbol{u}_k) - \mathcal{F}_k = 0 \qquad \text{in } V^*. \tag{8}$$

This solution strategy can be further refined by replacing the computation of $\mathcal{C}(\boldsymbol{u}_{k-1})$ with the current nonlinear iterate $\mathcal{C}(\boldsymbol{u}_k^m)$, resulting in a Newton-Rapson iteration scheme, in which the fully implicit nonlinear system (3) is resolved by replacing the exact Jacobian in equation (5) by an approximation in which $D_{\boldsymbol{u}}\mathcal{C}(\boldsymbol{u}_k^m)\dot{\boldsymbol{u}}_k$ is neglected, i.e.

$$D_{\boldsymbol{u}}\mathcal{R}(\boldsymbol{u}_k^m) \sim c_0\mathcal{M} - c_1\mathcal{C}(\boldsymbol{u}_k^m) + D_{\boldsymbol{u}}\mathcal{P}(\boldsymbol{u}_k^m). \tag{9}$$

In our numerical experiments, we use a generalized α-scheme for the fully implicit solver for the coupled system, with inexact Jacobian given by the discrete version of (9) and compare different solution strategies.

Example We consider a cantilever plate surrounded by a very viscous fluid in three dimensions, clamped at the left edge and initially deformed with a static load at the tip. At time $t = 0$, the load is removed and the vibrations of the plate are observed by plotting the tip displacement. We compare the three different coupling approaches, i.e., the fully implicit (9), the semi-implicit (8), and the segregated approach (6). The results for the fully implicit and the semi-implicit approach are identical for all cases, while the segregated approach yields stable results only for the smallest time step, while strong spurious oscillations appear when the time step is increased. We highlight that the computational cost of the semi-implicit approach is the same as in the segregated approach, assembling the matrices of the fluid problem only once per time step, and, therefore, significantly less than in the fully implicit approach where the fluid problem matrices are assembled in each Newton iteration. Accordingly, the semi-implicit approach appears to be a very efficient alternative combining the cost-effectiveness of the segregated approach with the accuracy and stability of the fully implicit approach.

References

[1] Luca Heltai, Marino Arroyo, and Antonio DeSimone. Nonsingular isogeometric boundary element method for Stokes flows in 3D. *Computer Methods in Applied Mechanics and Engineering*, 268:514–539, jan 2014.

[2] J. Kiendl, K.-U. Bletzinger, J. Linhard, and R. Wüchner. Isogeometric shell analysis with Kirchhoff–Love elements. *Computer Methods in Applied Mechanics and Engineering*, 198(49-52):3902–3914, nov 2009.

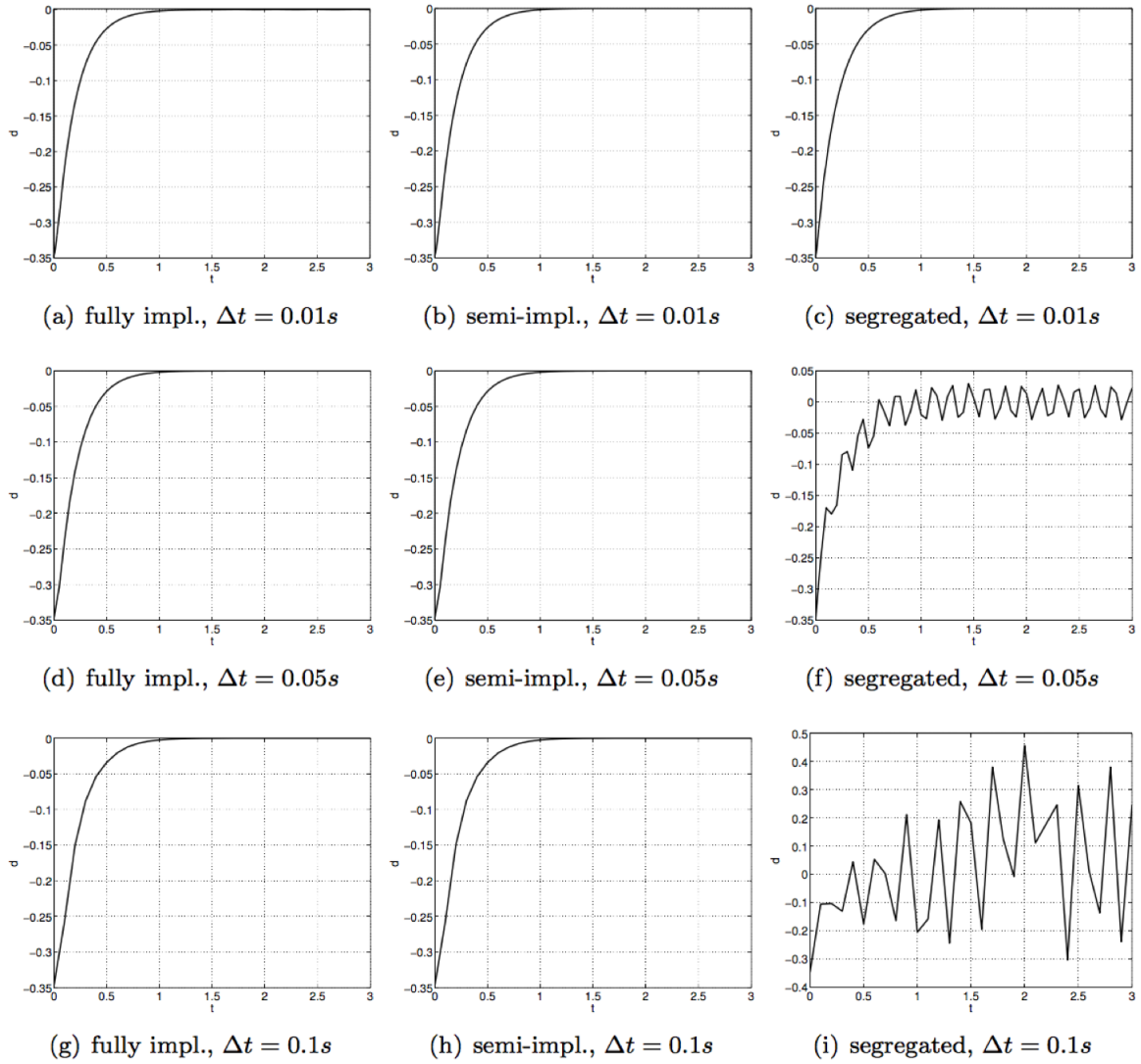


Figure 1: Vibration of a cantilever. Tip displacement for $\eta = 10$ using different coupling approaches and different time steps: fully implicit (left), semi-implicit (middle), segregated (right), with time steps $\Delta t = \{0.01, 0.05, 0.1\}s$ (top, middle, bottom).

[3] Josef Kiendl, Ming Chen Hsu, Michael C H Wu, and Alessandro Reali. Isogeometric Kirchhoff-Love shell formulations for general hyperelastic materials. *Computer Methods in Applied Mechanics and Engineering*, 291:280–303, 2015.

Algorithms for adaptive isogeometric methods using hierarchical splines, with an implementation in GeoPDEs

Rafael Vázquez
Istituto di Matematica Applicata e Tecnologie Informatiche "E. Magenes" del CNR
via Ferrata 1, 27100 - Pavia (Italy)
vazquez@imati.cnr.it

Eduardo Mario Garau
Instituto de Matemática Aplicada del Litoral (UNL, CONICET, FIQ), Santa Fe, Argentina
Santa Fe (Argentina)
egarau@santafe-conicet.gov.ar

One of the most active research topics on isogeometric analysis (IGA) is the development of adaptive methods for local refinement and coarsening. These methods require the use of spline spaces that go beyond the traditional tensor product structure. Several alternatives have been already proposed in the IGA community, such as T-splines, hierarchical splines, LR-splines or PHT-splines. Among them, hierarchical splines are probably the easiest to define and to implement, due to their multilevel structure.
In this work we introduce a set of structures and algorithms for the implementation of adaptive IGA methods based on hierarchical splines. Two main structures are defined: one for the hierarchical mesh, and one for the hierarchical basis. They rely on analogous structures for the tensor product spaces of each level, plus some methods related to the support of the basis functions. Methods to relate elements and functions of two consecutive levels are also required. With the help of these methods, we introduce algorithms to update the sets of active elements and basis functions during refinement and coarsening, which can be done either marking elements of the mesh or marking basis functions. The advantage of our algorithms with respect to [1] is that only local information is used during the update of the active sets. Moreover, the structures we define are simpler than those in [2], because mesh refinement is applied to the elements of the mesh, and no information about vertices is required.
All the algorithms have been implemented in the open source Octave (and Matlab) software GeoPDEs [3], and will be added to the package in a future release.

References

[1] Bornemann, P. B. and Cirak, F. 2013 *A subdivision-based implementation of the hierarchical B-splines finite element method*. Comput. Methods Appl. Mech. Engrg., 253, 584–598.

[2] Scott, M. A., Thomas, D. C. and Evans, E. J. 2014 *Isogeometric spline forests*. Comput. Methods Appl. Mech. Engrg., 269, 222–264.

[3] Vázquez, R. 2016 *A new design for the implementation of isogeometric analysis in Octave and Matlab: GeoPDEs 3.0*. IMATI Report Series, 16-02.

IGATOOLS: a general purpose C++14 library for Isogeometric Analysis

Massimiliano Martinelli
IMATI "E. Magenes" - CNR
via Ferrata, 5 27100 - Pavia Italy
martinelli@imati.cnr.it

Pablo Antolin
Dipartimento di Matematica "F. Casorati", Università degli Studi di Pavia
via Ferrata, 5 27100 - Pavia Italy
pablo.antolinsanchez@unipv.it

M. Sebastián Pauletti
Instituto de Matemática Aplicada del Litoral (IMAL), Consejo Nacional de Investigaciones científicas y técnicas (CONICET) and Universidad Nacional del Litoral
Santa Fe, Argentina
pauletti@santafe-conicet.gov.ar

We present the design and the implementation of IGATOOLS [1] (`http://www.igatools.org`), a C++14 general purpose library for solving PDEs using the isogeometric analysis framework [2].
In the IGATOOLS design, the mathematical concepts of the isogeometric method and their relationships are directly mapped into classes and their interactions. This encapsulation gives flexibility to use the library in a wide range of scientific areas and applications. We provide a precise framework for a lot of loose, available information regarding the implementation of the isogeometric method, and also discuss the similarities and differences between this and the finite element method.
The library uses advanced object oriented and generic programming techniques to ensure reusability, reliability, and maintainability of the source code. Among other capabilities, the library supports the development of dimension independent code (including manifolds and tensor-valued spaces), implements mutlithreaded methods and takes full advantage of the underlying tensor-product structure of the problem at hand (if any). The library also provides a plugin for interfacing with ParaView [3] in order to help the user to visualize the results.
We finally present a number of code examples to illustrate the flexibility and power of the library.

References

[1] M. S. Pauletti, M. Martinelli, N. Cavallini, and P. Antolin, "Igatools: An Isogeometric Analysis Library", *SIAM J. Sci. Comput.* (2015), **37(4)**, 465–496.

[2] T. J. R. Hughes, J. A. Cottrell, Y. Bazilevs, "Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement", *Comput. Methods Appl. Mech. Engrg.* (2005), **194**:39-41, 4135–4195.

[3] www.paraview.org

Statistical and numerical techniques for the analysis of complex biomedical signals

PROPOSERS

Anna Maria Paganoni
Politecnico di Milano
Pzza Leonardo da Vinci, 32 20133 - Milano Italy
anna.paganoni@polimi.it

Laura M. Sangalli
Politecnico di Milano
Pzza Leonardo da Vinci, 32 20133 - Milano Italy
laura.sangalli@polimi.it

SPEAKERS

Juan Romo (keynote)
Department of Statistics, Universidad Carlos III de Madrid
juan.romo@uc3m.es

Jean-Frédéric Gerbeau
Centre de Recherche Inria de Paris
jean-frederic.gerbeau@inria.fr

Luigi Ippoliti
Dipartimento Di Economia, Università degli Studi di Chieti - Pescara
luigi.ippoliti@unich.it

Alessandra Micheletti
Dipartimento di Matematica, Università degli Studi di Milano
Alessandra.Micheletti@unimi.it

Alessandro Vietti
ALPs - Alpine Laboratory of Phonetics and Phonology, Free University of Bozen
alessandro.vietti@unibz.it

The minisymposium focuses on the analysis of complex biomedical data, generated by medical scanners and devices. Both statistical and numerical methods will be presented.

Statistical techniques for the analysis of complex biomedical signals

Juan Romo
Department of Statistics, Universidad Carlos III de Madrid
juan.romo@uc3m.es

Statistical techniques for the analysis of complex biomedical signals.

A moment-matching method to study the variability of phenomena described by Partial Differential Equations

Jean-Frédéric Gerbeau
Centre Inria de Paris
2 rue Simone Iff, 75012 Paris, France
jean-frederic.gerbeau@inria.fr

Damiano Lombardi
Centre Inria de Paris
2 rue Simone Iff, 75012 Paris, France
damiano.lombardi@inria.fr

Eliott Tixier
Centre Inria de Paris
2 rue Simone Iff, 75012 Paris, France
eliott.tixier@inria.fr

Many phenomena are modeled by deterministic differential equations, whereas the observation of these phenomena, in particular in life science, exhibit an important variability. This work addresses the following question: how the model can be adapted to reflect the observed variability?
Given an adequate model, it is possible to account for this variability by allowing some parameters to adopt a stochastic behavior. Finding the parameters' probability density function that explains the observed variability is a difficult stochastic inverse problem, especially when the computational cost of the forward problem is high. In our approach, a non-parametric and non-intrusive procedure based on offline computations of the forward model is proposed. It infers the probability density function of the uncertain parameters from the matching of the observable statistical moments at different points in the physical domain. This inverse procedure is improved by incorporating a point selection algorithm that both reduces its computational cost and increases its robustness. This algorithm uses the pre-computed model outputs to build an approximation of the local sensitivities. The points in the physical domain are selected so that the maximum information on the sensitivities is conserved. The proposed approach is illustrated with a variety of ODE and PDE models, in particular in cardiac electrophysiology.

Hierarchical Dynamic Models for Structurally Nested Biomedical Signals

Luigi Ippoliti
Università degli Studi di Chieti-Pescara, DMQTE
viale Pindaro, 42 65125 - Pescara Italy
ippoliti@unich.it

Alexandra M. Schmidt
Departamento de Métodos Estatísticos, UFRJ
Rio de Janeiro, Brazil
alex@im.ufrj.br

Josiane S. C. Coelho
Universidade Federal Rural do Rio de Janeiro
Rio de Janeiro, Brazil
e-mailaddress

Helio S. Migon
Departamento de Métodos Estatísticos, UFRJ
Rio de Janeiro, Brazil
alex@im.ufrj.br

Modern biomedical instrumentation and acquisition technologies generate large data sets collecting various measurements describing for example brain activities, tissues, or cells. Recently, the development of computer applications in the field of life sciences, in particular for the clinical and biomedical environments, has also gained increasing attention due to the promising results in the treatment of patients. In fact, potential applications in the biomedical field include the construction of diagnostic or prognostic rules which, in general, appear hardly possible without the help of efficient statistical and computing techniques.

Biomedical applications using multivariate statistical techniques is a major area of interest that has been investigated by a large number of scientific researchers. Biomedical signals originate from a variety of sources and in many experiments these signals come to us through a process naturally described as functional.

An important task when analyzing such data is to extract the essential information representative of the underlying biological or biophysical processes. However, there is no single approach which can be considered uniformly as being the most appropriate solution for a specific problem. The choice of the approach is generally dictated by the objective of the study, whether it be estimating trends, obtaining forecasts of the signals, or increasing the scientific understanding of the underlying mechanisms.

The focus of this work is to provide a reliable modelling approach for fitting curves, in the form of biomedical time series, that share a strong physical relationship. In general, there are several features which should be considered when modelling families of signals. Those which are relevant for our work refer to: (a) the characterization of an average or a

typical time course, (b) the fit of individual signals from noisy data, (c) the study of the existing variability among the time series, (d) the characterization of the nested hierarchy of the series, and (e) the modelling of the serial correlation for each series, as well as the correlation existing among the series.
The theoretical development of the last two points represents an important methodological part of our work. In general, the estimation of covariance structures appears a difficult problem. This is not an exception in our case study, where we also consider the additional problem of parameterizing the covariance matrix for a set of replicated signals with a hierarchical structure and that are also correlated at their deepest possible level.
The work is motivated by the study of the so called Raynaud's Phenomenon - RP. This is a paroxysmal vasospastic disorder of small arteries, pre-capillary arteries and cutaneous arteriovenous shunts of extremities, typically induced by cold exposure and emotional stress. RP can be classified as primary (PRP), with no identifiable underlying pathological disorder, or secondary (SS), usually associated with a connective tissue disease, the use of certain drugs, or the exposition to toxic agents.
We propose a hierarchical dynamic Gaussian model (HDLM) which is able to describe the hierarchical nature of the data as well as their temporal dynamics, both for single individuals and for the three groups (control, RP and SS) under study. Many of the estimated model parameters have also a direct interpretation and are helpful to describe specific features of RP. Our proposed model and inference procedure naturally provide the predictive likelihood of a new individual belonging to one of the three groups under study, which is another important aspect of this analysis. To the best of our knowledge, our work represents the first attempt at a rigorous statistical modelling strategy of the dynamics of the different forms of RP.

Statistical geometric methods for fibre processes modelling biomedical problems

Alessandra Micheletti
Università degli Studi di Milano
Dip. di Matematica, via Saldini, 50 20133 - Milano Italy
alessandra.micheletti@unimi.it

Statistical methods related with stochastic geometries, and in particular with fibre processes, can be applied to address a big set of biomedical problems, ranging from quantifying dose/effect ratios in medical treatments, to automatic diagnosis of pathologies related with the *shape* of the fibre process under study, whose description can be highly complex. In this context, statistical methods based on suitable descriptors of the geometry of the fibre process are needed to compare quantitatively patterns arising in different experimental or pathological conditions, also taking into account spatial heterogeneities of the patterns, which are very frequent in real applications [1].
Fibre processes are also used to model dynamic phenomena like angiogenesis, vasculogenesis, formation of neuronal networks, etc. In such cases some of the stochastic dynamical models available in literature [2, 3] describe the evolution of tips of vessels, coupled with the evolution of some underlying fields of nutrients. The parameters of these models are strictly connected with the geometry of the generated vessels. Statistical techniques for parameter estimation of such models, based on suitable descriptors of the geometry of the fibres, are needed to validate the models themselves.
In this talk we will address some of these problems and provide some first proposals of solutions, based on computational statistical techniques. Different geometric descriptors of the fibre processes will be tested, and the properties of the proposed parameter estimators will be studied on simplified simulated test cases.

References

[1] A. Micheletti , V. Capasso, Statistical methods for the analysis of stochastic fibre processes, in *Proceedings of the workshop Integrated multidisciplinary approaches in the study and care of the human eye. Clinical experience, mathematical modelling, new technologies*. Causin, Guidoboni, Harris, Sacco Eds, Kugler Publications, Amsterdam, The Netherlands, 2014.

[2] V. Capasso, D. Morale, G. Facchetti, The role of stochasticity in a model of retinal angiogenesis. In *IMA Journal of Applied Mathematics*, 77 (6), pp.729-747, 2012.

[3] V. Capasso, D. Morale, G. Facchetti, Randomness in self-organized phenomena. A case study: retinal angiogenesis. *Biosystems*, 112 (3), pp.292-297, 2013.

Functional data analysis of tongue movements

Alessandro Vietti
ALPS - Alpine Laboratory of Phonetic Sciences
Libera Università di Bolzano
Piazza Università, 1 39100 - Bolzano Italy
alessandro.vietti@unibz.it

Alessia Pini
MOX Laboratory for Modeling and Scientific Computing
Dept. of Mathematics - Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
alessia.pini@polimi.it

Simone Vantini
Dept. of Mathematics - Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
simone.vantini@polimi.it

Lorenzo Spreafico
ALPS - Alpine Laboratory of Phonetic Sciences
Libera Università di Bolzano
Piazza Università, 1 39100 - Bolzano Italy
lorenzo.spreafico@unibz.it

In the last decades, functional data analysis (FDA) techniques have been successfully applied to the analysis of biologic [5] and human movements data [4]. In speech production research, ultrasound imaging of the tongue is increasingly pervasive. Different methods have been proposed so far regarding the quantification and statistical analysis of ultrasound data [1]. SSANOVA (smoothing spline ANOVA), a parametric approach based on Bayesian inference, has been extensively applied as a standard method to compare set of tongue curves [2]. In linguistic studies, researchers may want to determine whether the tongue shape for an articulation under two different conditions (e.g., consonants in word-initial versus word-medial position) is the same or different. In this talk we will illustrate how IWT [3], a novel method of functional data analysis, can be applied to the comparison of tongue curves. The technique is applied to a dataset of tongue shapes recorded for a study on bilingual speech (German and Italian in South Tyrol, [6]). We test differences in the production of similar sequences of sounds in the two languages spoken by bilingual speakers (e.g. *tra* as in the German word *tragen* 'to bring' and in the Italian word *trave* 'beam'). The output of the IWT is an adjusted p-value function that can be used to select intervals of the domain imputable for the rejection of a null hypothesis. IWT is jointly applied to the position, slope, and concavity of the tongue profiles. IWT-based comparisons result in an informative and detailed representation of the regions of the tongue where a significant difference is located.

References

[1] Davidson, L. 2006 *Comparing tongue shapes from ultrasound imaging using smoothing spline analysis of variance.* Journal of the Acoustical Society of America 120(1), 407-415.

[2] Gu, C. 2002 *Smoothing Spline ANOVA models.* New York, Springer.

[3] Pini, A. and Vantini, S. 2015 *Interval-wise testing for functional data.* Technical Report 30/2015, MOX – Department of Mathematics, Politecnico di Milano.

[4] Ramsay, J. O., Gribble, P., and Kurtek, S. 2014 *Description and processing of functional data arising from juggling trajectories.* Electronic Journal of Statistics 8(2), 1811-1816.

[5] Sangalli, L. M., Secchi, P. Vantini, S. 2014 *AneuRisk65: A dataset of three-dimensional cerebral vascular geometries.* Electronic Journal of Statistics 8(2), 1879-1890.

[6] Vietti, A. and Spreafico, L. 2015 *An ultrasound study of the phonetic allophony of Tyrolean /r/.* ICPhS 2015 Proceedings.

Complex data with spatial dependence

PROPOSERS

Anna Maria Paganoni
Politecnico di Milano
Pzza Leonardo da Vinci, 32 20133 - Milano Italy
anna.paganoni@polimi.it

Laura M. Sangalli
Politecnico di Milano
Pzza Leonardo da Vinci, 32 20133 - Milano Italy
laura.sangalli@polimi.it

SPEAKERS

Alessandro Fassò (keynote)
Dipartimento di Ingegneria gestionale, dell'informazione e della produzione, Università degli Studi di Bergamo
alessandro.fasso@unibg.it

Alberto Guadagnini
Dipartimento di Ingegneria Civile e Ambientale, Politecnico di Milano
alberto.guadagnini@polimi.it

Rosaria Ignaccolo
Dipartimento di Economia e Statistica, Università degli Studi di Torino
rosaria.ignaccolo@unito.it

Alessandra Menafoglio
Dipartimento di Matematica, Politecnico di Milano
alessandra.menafoglio@polimi.it

Davide Pigoli
Department of Pure Mathematics and Mathematical Statistics, University of Cambridge
dp497@statslab.cam.ac.uk

The minisymposium focuses on the analysis of complex data with spatial dependence, presenting both methodological advances and applications in the domains of earth and environmental sciences.

Advanced statistical applications of complex data indexed in space and time

Alessandro Fassò
Università degli Studi di Bergamo
viale Marconi, 5, 2044 - Dalmine Italy
alessandro.fasso@unibg.it

In this talk, I will review some applications based on spatio-temporal modelling and functional data. Applications are related to air quality, atmospheric sciences and health surveillance of medical devices.

Regarding air quality, following [1, 6, 4] will consider the distribution of population by exposure to multiple airborne pollutants, taking into account the spatio-temporal variability of air quality and the spatial spread of human population across Europe. From the technical point of view the complexity of statistical modelling must take into account the dataset size in order to be computationally feasible, without loosing important details. In particular, we consider monitoring network data for five pollutants, namely carbon monoxide, nitrogen dioxide, ozone, coarse and fine particulate matters. In order to optimize the spatial information content and to allow the computation of daily multi-pollutant exposure distributions across space and time, we introduce a multivariate spatio-temporal model which is estimated using the EM algorithm and allows us to estimate daily multipollutant concentration in high spatial resolution. As a result we compare the daily population exposure of 33 European countries and three important metropolitan areas in years 2009-2011.

In climate monitoring, the quantification of measurement uncertainty of atmospheric parameters is a key factor in assessing the uncertainty of global change estimates given by numerical prediction models, [5, 2]. One of the critical contributions to the uncertainty budget is related to the collocation mismatch in space and time among observations made at different locations. This is particularly important for vertical atmospheric profiles obtained by radiosondes. In this talk, I will review a statistical modelling approach capable of explaining the relationship between collocation uncertainty and a set of environmental factors, height and distance between imperfectly collocated trajectories. The new statistical approach is based on the heteroskedastic functional regression (HFR) model which extends the standard functional regression approach and allows a natural definition of uncertainty profiles. Along this line, a five-fold decomposition of the total collocation uncertainty is proposed, giving both a profile budget and an integrated column budget.

Functioning of high tech medical devices, such as surgery sterilizers, is often characterized by a set of measurements profiles collected in high frequency. Hence health surveillance of the device can be based on control charts for functional objects, [3]. In this talk, I will introduce a general functional exponential weighted moving average control chart (f-EWMA). Moreover I will show that when functional data to be monitored are smooth enough to be representable by a finite dimensional basis, a particular version of these functional EWMA's is shown to be a multivariate EWMA applied to basis expansion coefficients. The use of f-MEWMA is illustrated in connection to health monitoring of a

steam sterilizer during its life cycle. Indeed, each sterilization run gives several profiles related to machine health and degradation of the steam sterilizer during its life cycle modifies profile curvature in an unpredictable way.

References

[1] Fassò, A, Finazzi F, Ndongo F. (2016) *European population exposure to airborne pollutants based on a multivariate spatio-temporal model*. Submitted.

[2] Fassò, A, Ignaccolo, R, Madonna, F, Demoz, B. and Franco-Villoria M. (2014) *Statistical modelling of collocation uncertainty in atmospheric thermodynamic profiles*, Atmos. Meas. Tech., 7, 1803-1816.

[3] Fassò, A, Toccu M. Marino M. (2016) *Functional Control Charts and Health Monitoring of Steam Sterilizers*. Quality and Reliability Engineering International. In printing.

[4] Finazzi F, Haggarty R, Miller C, Scott M, Fassò A. (2015) *A comparison of clustering approaches for the study of the temporal coherence of multiple time series*. Stochastic Environmental Research and Risk Assessment. Volume 29, Issue 2, 463-475.

[5] Ignaccolo R, Franco-Villoria M, Fassò A. (2015) *Modelling collocation uncertainty of 3D atmospheric profiles*. Stochastic Environmental Research and Risk Assessment. 29 (2), 417-429.

[6] Finazzi F, Fassò A. (2014) *D-STEM: A Software for the Analysis and Mapping of Environmental Space-Time Variables*. Journal of Statistical Software. Vol. 62, Issue 6, 1-29.

A Geostatistical Scaling Approach for the Analysis of Non Gaussian Random Variables and Increments

Alberto Guadagnini
Dipartimento di Ingegneria Civile e Ambientale, Politecnico di Milano
Piazza L. Da Vinci, 32 20133 - Milano Italy
alberto.guadagnini@polimi.it

Monica Riva
Dipartimento di Ingegneria Civile e Ambientale, Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
monica.riva@polimi.it

Shlomo P. Neuman
Department of Hydrology and Atmospheric Sciences, University of Arizona
Tucson, Arizona 85721, USA
neuman@hwr.arizona.edu

We address manifestations of non-Gaussian statistical scaling displayed by many environmental variables, Y, and their (spatial or temporal) increments. Evidence of such behavior includes symmetry of increment distributions at all separation distances (or lags) with sharp peaks and heavy tails which tend to decay asymptotically as lag increases. Variables reported to exhibit such distributions include quantities of direct relevance to hydrogeological and environmental sciences, e.g. porosity, log permeability, electrical resistivity, soil and sediment texture, sediment transport rate, and other. We discuss the way our recently proposed generalized sub-Gaussian model (GSG) can reconcile within a unique theoretical framework the probability distributions of a target variable and its increments. We show and discuss expressions for probability distribution functions of Y and its increments as well as their lead statistical moments. We then demonstrate the feasibility of estimating all key parameters of our GSG model by analyzing jointly spatial moments of Y data and corresponding increments. We do so by relying on synthetic examples as well as neutron porosity data associated with deep boreholes in reservoirs.

Functional Kriging Uncertainty Assessment

Rosaria Ignaccolo
Università degli Studi di Torino
Lungo Dora Siena 100A, 10153 - Torino Italy
rosaria.ignaccolo@unito.it

Maria Franco-Villoria
Università degli Studi di Torino
Lungo Dora Siena 100A, 10153 - Torino Italy
maria.francovilloria@unito.it

Geostatistical techniques for functional data were introduced by Goulard and Voltz (1993) [4], but have only been developed recently. Several papers consider ordinary and universal kriging models to predict a curve at an unmonitored site under the assumption of a constant or longitude and latitude dependent mean (see e.g. [2, 3, 8, 1, 7]) or kriging with external drift [5], where scalar and functional exogenous variables are introduced. However, uncertainty evaluation of a predicted curve remains an open issue. Given the difficulty to derive sampling distributions for functional data, prediction band derivation can be approached using resampling methods. To evaluate uncertainty of a predicted curve, we adapt two semi-parametric bootstrap approach for spatially correlated data proposed by [10] and [6] to the functional data case. The approach is illustrated by means of a simulation study.

1 Functional Kriging with External Drift (FKED)

Let $\Upsilon_s = \{Y_s(t); t \in T\}$ be a functional random variable observed at location $s \in D \subseteq \mathbb{R}^d$, whose realization is a function of $t \in T$, T compact subset of $\mathbb{R}$. Assume that we observe a sample of curves Υ_{s_i}, for $s_i \in D$, $i = 1, \ldots, n$, that take values in a separable Hilbert space of square integrable functions. The set $\{\Upsilon_s, s \in D\}$ constitutes a functional random field or a *spatial functional process* [2], that can be non-stationary and whose elements are supposed to follow the model $\Upsilon_s = \mu_s + \epsilon_s$. The term μ_s is interpreted as a drift describing a spatial trend while ϵ_s represents a residual random field that is zero-mean, second-order stationary and isotropic. At the generic site s_i, $i = 1, \ldots, n$, and at point t, the model can be rewritten as a functional concurrent linear model $Y_{s_i}(t) = \mu_{s_i}(t) + \epsilon_{s_i}(t)$ with the drift

$$\mu_{s_i}(t) = \alpha(t) + \sum_p \gamma_p(t) C_{p,i} + \sum_q \beta_q(t) X_{q,i}(t) \tag{1}$$

where $\alpha(t)$ is a functional intercept, $C_{p,i}$ and $X_{q,i}$ are the p^{th} and q^{th} scalar and functional covariates at site s_i with coefficients $\gamma_p(t)$ and $\beta_q(t)$ and $\epsilon_{s_i}(t)$ represents the residual spatial functional process $\{\epsilon_s(t), t \in T, s \in D\}$ at site s_i. Once the Functional Regression Model (1) has been fitted by means of a GAM representation (for details see [5]), the functional residuals $e_{s_i}(t) = Y_{s_i}(t) - \hat{\mu}_{s_i}(t)$ can be used to predict the residual curve at a new site s_0 via ordinary kriging for functional data [3], according to which $\hat{e}_{s_0}(t) =$

Work supported by "Futuro in Ricerca" 2012 Grant (project no. RBFR12URQJ) provided MIUR.

$\sum_{i=1}^{n} \lambda_i e_{s_i}(t)$, with $\lambda_i \in \mathbb{R}$. Prediction at the new site s_0 is obtained by adding up, as in the classical regression kriging, the two terms, i.e. $\hat{Y}_{s_0}(t) = \hat{\mu}_{s_0}(t) + \hat{e}_{s_0}(t)$, where $\hat{\mu}_{s_0}(t) = \hat{\alpha}(t) + \sum_p \hat{\gamma}_p(t) C_{p,0} + \sum_q \hat{\beta}_q(t) X_{q,0}(t)$ depends on the covariate values $C_{p,0}$ and $X_{q,0}(\cdot)$ at the site s_0.

2 Uncertainty evaluation

To evaluate the uncertainty of a predicted curve $\hat{Y}_{s_0}(t)$ at a new site s_0, we consider two semi-parametric bootstrap approaches for spatially correlated data proposed by [10] and [6] and extend them to the functional context. Suppose that $\hat{Y}_{s_0}(t) - Y_{s_0}(t)$ follows the distribution F_n, a $1-\alpha$ prediction interval for $Y_{s_0}(t)$ can be built as $(\hat{Y}_{s_0}(t) - q_{1-\alpha/2}, \hat{Y}_{s_0}(t) - q_{\alpha/2})$, with q_α the α^{th}-quantile of the unknown distribution F_n. The idea is to construct B bootstrap replicates $\{\hat{Y}^{*j}_{s_0}, Y^{*j}_{s_0}\}_{j=1}^{B}$ and approximate F_n by $\hat{F}^*_n$, the empirical distribution of $\{\hat{Y}^{*j}_{s_0} - Y^{*j}_{s_0}\}_{j=1}^{B}$. The bootstrapping algorithm can be summarized as follows:

1. Estimate and remove the drift following Model (1) to obtain $\epsilon_{s_i}(t) = Y_{s_i}(t) - \hat{\mu}_{s_i}(t)$.

2. Estimate the functional residuals covariance matrix Σ through the estimated trace-semivariogram:

$$\hat{v}(h) = \frac{1}{2\,|N(h)|} \sum_{i,j \in N(h)} \int_T \left(e_{s_i}(t) - e_{s_j}(t)\right)^2 dt$$

   where $N(h) = \{(s_i, s_j) : \|s_i - s_j\| = h\}$. A parametric model (e.g. Matérn) can be fitted to the points $(h_g, \hat{v}(h_g)), g = 1, \ldots, G$, as in classical geostatistics. Using Cholesky decomposition, $\hat{\Sigma} = \hat{L}\hat{L}^T$ and the functional residuals can be transformed:

$$\zeta_{n\times M} = (\zeta(s_1), \ldots, \zeta(s_n))' = \hat{L}^{-1}_{n\times n} \left(Y_{n\times M} - \hat{\mu}_{n\times M}\right).$$

3. Generate B bootstrap samples with size $n+1$, $\zeta^*_{n+1} = (\zeta^*(s_1), \ldots, \zeta^*(s_n), \zeta^*(s_{n+1}))'$ from $\zeta(s_1), \ldots, \zeta(s_n)$.

4. Create the augmented covariance matrix $\hat{\Lambda} = \begin{bmatrix} \hat{\Sigma} & \hat{c}_n^T \\ \hat{c}_n & \hat{\sigma}^2 \end{bmatrix}$, where $\hat{c}_n = \{\hat{C}(s_i - s_0)\}_{i=1}^{n}$, $\hat{C}$ is the estimated covariance function and $\hat{\sigma}^2 = \hat{C}(0)$ is the estimated sill. Use Cholesky decomposition so that $\hat{\Lambda} = \hat{R}\hat{R}^T$ and transform the bootstrap samples ζ^*_{n+1} as

$$(e^*(s_1), \ldots, e^*(s_n), e^*(s_0))' = \hat{R}_{(n+1)\times(n+1)} \zeta^*_{(n+1)\times M}.$$

5. The final bootstrap sample is determined as $Y^*_{s_i}(t) = \hat{\mu}_{s_i}(t) + e^*_{s_i}(t)$, $i = 1, \ldots, n$ and $Y^*_{s_0}(t) = \hat{\mu}_{s_0}(t) + e^*_{s_0}(t)$.

The bootstrap samples $\{Y^{*j}_{s_1}, \ldots, Y^{*j}_{s_n}\}_{j=1}^{B}$ are then fed into the FKED method to obtain B prediction curves $\hat{Y}^{*j}_{s_0}$ and the differences $\{\hat{Y}^{*j}_{s_0} - Y^{*j}_{s_0}\}_{j=1}^{B}$ are considered. The prediction interval for $Y_{s_0}(t)$ can be written as $(\hat{Y}_{s_0}(t) - q^*_{1-\alpha/2}, \hat{Y}_{s_0}(t) - q^*_{\alpha/2})$, with q^*_α the α-percentile of $\hat{F}^*_n$, that can be obtained ordering the curves. There is no gold standard for ordering functional data. Here we consider two ordering techniques based on band depth and L^2 distance. Band depth [9] can be defined for any set of k curves (here $k = 2$). The sample band depth (BD) of $y(t)$ can be calculated as the proportion of bands delimited by two

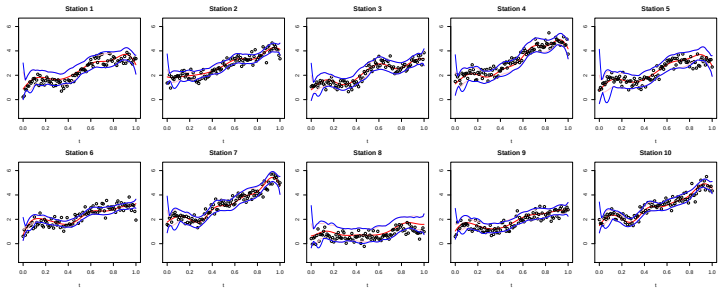


Figure 1: Original data (black dots), FKED predicted curve (solid red line), 95% prediction band (pink) based on L^2 distance (pink) and on *MBD* (blue) for $n = 50$, $\sigma^2 = 0.25$, $\phi = 1.5$.

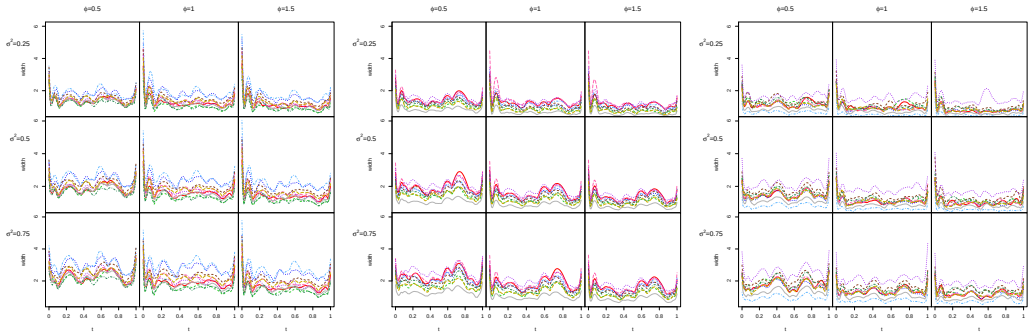


Figure 2: Band width (depth) for $n = 25$ (left), $n = 50$ (middle) and $n = 90$ (right).

curves containing the whole curve $y(t)$ [9]; here we use the modified band depth (*MBD*), that takes into account whether a portion of the curve is in the band (for details see [9]). The lower/upper limits of a (depth based) 95% prediction band are obtained by taking the pointwise (w.r.t. t) minimum/maximum of the 95% deepest curves (in the case of band depth) or of the 95% curves closest to the zero curve (in the case of using L^2 distance)

3 Simulation study

We aim to analyse the impact that trend complexity, spatial structure (via the covariance function parameters of the functional residual random field) and ordering technique have on the performance of the bootstrapping method when increasing the number of sites. Data were simulated using cubic B-splines on a spatial irregular grid (n locations) on $D = [0, 2] \times [0, 3]$ and curve domain $T = [0, 1]$. The residual functional random field was built as $e_s(t) = \sum_{j=1}^{10} \xi_j(s) B_j(t)$, where $B_j(t)$ is the j^{th} basis function evaluated at $t \in T$. The spatially correlated spline coefficients $\{\xi_j(s), s \in D\}$ were generated for each j in $1, \ldots, 10$ using the same exponential covariance function with range and scale parameters $\phi \in (0.5, 1, 1.5)$ and $\sigma^2 \in (0.25, 0.50, 0.75)$ respectively, resulting in 9 different scenarios. The drift was obtained as $m_s(t) = \alpha(t) + \beta_1(t) lon + \beta_2(t) lat$, where lon and lat are the spatial coordinates, $\alpha(t)$ is a functional intercept and $\beta_1(t), \beta_2(t)$ are functional coefficients that can be expressed in terms of B-spline basis (whose coefficients can be chosen to determine the complexity of the drift). Finally, simulated observations were built as

$$Y_s^{sim}(t) = m_s(t) + e_s(t) + \xi_s(t)$$

where $\xi(t) = \{\xi_{s_1}(t), \ldots, \xi_{s_n}(t)\} \sim N_n(0, 0.09)$ is a vector of random errors for each fixed $t \in [0, 1]$. For each simulation scenario, we generated functional data at $n = 25, 50$ and 90 nested locations. Additionally data were generated at 10 more sites used as validation stations. The FKED model (Section 1) was applied to each simulated data set to predict curves at the 10 validation sites. For each validation station $B = 500$ predictions were obtained following Section 2 and 95% prediction bands were produced using both distance and *MBD*. An example can be seen in Figure 1. To evaluate the performance of the proposal, we consider two different indicators: the width of the resulting 95% prediction interval and the proportion of the simulated curve within the interval. Figure 2 summarizes (depth) band width for all sample sizes and simulation scenarios. As one would expect, band width decreases with increasing sample size. Moreover, band width increases with increasing σ^2 and decreases slightly with increasing ϕ for a fixed value of σ^2. The depth-based band is practically always wider than the distance-based one. In terms of coverage (figure not shown here), the performance appears good and improves with increasing sample size.

4 Discussion

We propose a semi-parametric bootstrap approach that allows the construction and evaluation of simultaneous prediction bands - over T - for the functional kriging predictor with a non-constant width. The simulation study shows that the proposed technique has a good performance. We are currently investigating the effect of more complex drifts as well as alternative ways of evaluating the performance of the proposal.

References

[1] Caballero, W., Giraldo, R. and Mateu, J. 2013 *A universal kriging approach for spatial functional data*. Stoch. Env. Res. Risk Assess. 27(7), 1553–1563.

[2] Delicado, P., Giraldo, R., Comas, C. and Mateu, J. 2010 *Statistics for spatial functional data: some recent contributions*. Environmentrics, 21, 224–239.

[3] Giraldo, R., Delicado, P. and Mateu, J. 2011 *Ordinary kriging for function-valued spatial data*. Environmental and Ecological Statistics, 18(3), 411–426.

[4] Goulard, M. and Voltz, M. 1993 Geostatistical interpolation of curves: A case study in soil science. In *Geostatistics Troia '92*(ed. A. Soares), vol. 2, pp. 805–816, Kluwer Academic, Dordrecht.

[5] Ignaccolo, R., Mateu, J. and Giraldo, R. 2014 *Kriging with external drift for functional data for air quality monitoring*. Stoch. Env. Res. Risk Assess. 28(5), 1171–1186.

[6] Iranpanah, N., Mohammadzadeh, M. and Taylor, C.C. 2011 *A comparison of block and semi-parametric bootstrap methods for variance estimation in spatial statistics*. Comput. Statist. Data Anal. 55, 578–587.

[7] Menafoglio, A., Secchi, P. and Dalla Rosa, M. 2013 *A Universal Kriging predictor for spatially dependent functional data of a Hilbert Space*. Electron. J. Stat. 7, 2209–2240.

[8] Nerini, D., Monestiez, P. and Manté C. 2010 *Cokriging for spatial functional data*. J. Multivariate Anal. 101, 409–418.

[9] Lopez-Pintado, S. and Romo, J. 2009 *On the concept of depth for Functional Data.* J. Amer. Statist. Assoc. 104(486), 718–734.

[10] Schelin, L. and Sjöstedt-de Luna, S. 2010 *Kriging prediction intervals based on semiparametric bootstrap.* Math. Geosci. 42, 985–1000

Geostatistical K-mean clustering for heterogeneous density functions in composite systems

Alessandra Menafoglio
Politecnico di Milano
p.zza Leonardo da Vinci 32 - Milano Italy
alessandra.menafoglio@polimi.it

Piercesare Secchi
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
piercesare.secchi@polimi.it

Alberto Guadagnini
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
alberto.guadagnini@polimi.it

The statistical analysis of Functional Compositions (FCs) is a key issue in Earth Sciences. Proper characterization of FCs is crucial to environmental applications for which available data can be treated as probability density functions.
In this communication, we investigate the problem of geostatistically characterizing the spatial heterogeneity of a set of particle-size density functions in a geological system composed by disjoint subdomains each associated with a different lithotype. We ascribe the heterogeneity of the system to a latent random field, which is associated with a grouping structure in the observed field of densities. We rest our developments on the theory of Bayes Hilbert spaces [1, 4], combined with the viewpoint of Functional Data Analysis. The former allows to cope with the data constraints, the latter enables one to overcome the curse of dimensionality which inevitably affects the (geo)statistical analysis of infinite-dimensional data. We revise the key concepts of clustering functional data in light of the Bayes space theory and develop an original K-means method for spatially dependent FCs. We rely on a geostatistical approach to estimate the spatial dependence, and show how to incorporate the clustering information into the geostatistical model, for the purpose of performing predictions via a Class-Kriging methodology [2].
We demonstrate the potential of the proposed method through a field scale application relying on a set of particle-size densities collected within a three-dimensional heterogeneous aquifer, which is conceptualized as a composite system associated with an uncertain spatial arrangement of geomaterials.

References

[1] Egozcue, J. J., Díaz-Barrero, J. L., Pawlowsky-Glahn V. 2006. Hilbert space of probability density functions based on Aitchison geometry. *Acta Mathematica Sinica*, English Series, 22(4):1175–1182.

[2] Menafoglio, A., Secchi, P., Guadagnini, A. 2016. A Class-Kriging predictor for Functional Compositions with application to particle-size curves in heterogeneous aquifers. *Mathematical Geosciences*, DOI: 10.1007/s11004-015-9625-7.

[3] Pawlowsky-Glahn, V., Buccianti, A. 2011. *Compositional data analysis. Theory and applications*. Wiley.

[4] van den Boogaart, K. G., Egozcue, J. J., Pawlowsky-Glahn, V., 2014. Bayes Hilbert spaces. *Australian & New Zealand Journal of Statistics*, 56:171–194, 2014.

Residual kriging for positive definite matrix-valued geostatistical data

Davide Pigoli
University of Cambridge
Wilberforce Road, Cambridge CB3 0WB, United Kingdom
dp497@cam.ac.uk

Alessandra Menafoglio
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
alessandra.menafoglio@polimi.it

Piercesare Secchi
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
piercesare.secchi@polimi.it

We describe here a kriging procedure for geolocalized data belonging to a Riemannian manifold. Spatial statistics for complex data has recently received much attention within the field of functional data analysis (see [2] and [5]) but the extension to non Euclidean data is even a greater challenge.
Previous works have considered the problem of dealing with independent manifold-valued response variables. Some of them propose non parametric or semi-parametric approaches but this implies a lack of interpretability or the reduction of multivariate predictors to univariate features. In particular, these approaches do not allow to introduce the spatial information in the prediction procedure.
We propose to use the local geometry of the manifold to find a data-driven linearization, i.e. looking for the tangent space where the parametric model provides the best possible fit for the available data. This local approach is similar to those advocated in [3] but allows us to include multiple covariates (for example, geographical coordinates) in the drift term. The method is illustrated here for the special case of positive definite symmetric matrices and in view of a meteorological application to covariance matrices. More in general, this approach is valid every time a Hilbert tangent space and correspondent logarithmic and exponential map can be defined (see [6]).

1 A tangent space model for kriging prediction

In this section we apply a regression approach based on local tangent space approximation to non-stationary random fields taking value in the space $PD(p)$ of positive definite symmetric matrices of order p. The main idea is to use a tangent space model to approximate the geometry of the manifold and to refer to the tangent space to deal with spatial dependence. Thus, the proposed model is the following: for $\mathbf{s} \in D \subset \mathbb{R}^d$,

$$S(\mathbf{s}; \boldsymbol{\beta}, \Sigma) = \exp_{\Sigma}(A(\mathbf{x}(\mathbf{s}); \boldsymbol{\beta}) + \Delta(\mathbf{s})), \tag{1}$$

where $\exp_\Sigma$ is the exponential map at Σ from $Sym(p)$ (the Euclidean space of symmetric matrices of order p) to $PD(p)$. $A(\mathbf{x}(\mathbf{s});\boldsymbol{\beta})$ is a parametric model depending on the covariates $\mathbf{x}(\mathbf{s})$ and unknown parameters $\boldsymbol{\beta}$ and Δ is a zero-mean, globally second-order stationary and isotropic random field taking values in $Sym(p)$. This means that $\mathbb{E}[\Delta(\mathbf{s})]$ is the null matrix for all $\mathbf{s}$ in D and, for $\mathbf{s}_i, \mathbf{s}_j \in D$, the covariance between $\Delta(\mathbf{s}_i)$ and $\Delta(\mathbf{s}_j)$ depends only on the distance between $\mathbf{s}_i$ and $\mathbf{s}_j$, i.e., $\text{cov}(\Delta(\mathbf{s}_i), \Delta(\mathbf{s}_j)) = C(||\mathbf{s}_i - \mathbf{s}_j||)$. This definition of the covariogram C follows the approach detailed in [5] for data belonging to Hilbert spaces. Equivalently, under the previous assumptions, for $\mathbf{s}_i, \mathbf{s}_j \in D$, the spatial dependence of the field can be represented by the semivariogram defined as $\gamma(||\mathbf{s}_i - \mathbf{s}_j||) = \frac{1}{2}\text{var}(\Delta(\mathbf{s}_i) - \Delta(\mathbf{s}_j)) = \frac{1}{2}\mathbb{E}[||\Delta(\mathbf{s}_i) - \Delta(\mathbf{s}_j)||_F^2]$, $||.||_F$ being the Frobenius norm. The assumption of isotropy can be relaxed but it brings additional complication in the estimation of the spatial dependence and this is outside of the scope of this work.

Let $\mathbf{s}_1, ..., \mathbf{s}_n$ be distinct locations in the domain D and assume that, in each location $\mathbf{s}_i$, the covariate vector $\mathbf{x}(\mathbf{s}_i)$ is observed together with a realization S_i of the random field (1). If the spatial dependence structure was known, the parameters of (1) could be estimated following the generalized least square approach detailed in [6].

If Σ and $\boldsymbol{\beta}$ were known, the spatial dependence of the random field Δ on the tangent space could be estimated in $Sym(p)$ by considering the residuals $\Delta(\mathbf{s}_i) = A(\mathbf{x}(\mathbf{s}_i);\boldsymbol{\beta}) - \log_\Sigma(S_i)$ as an incomplete realization of the random field Δ, $\log_\Sigma$ being the logarithmic map at Σ from $PD(p)$ to $Sym(p)$. Indeed, the empirical semivariogram in $Sym(p)$ could thus be estimated with the method of moments estimator proposed in [1],

$$\widehat{\gamma}(h) = \frac{1}{2|N(h)|} \sum_{(\mathbf{s}_i,\mathbf{s}_j)\in N(h)} ||\Delta(\mathbf{s}_i) - \Delta(\mathbf{s}_j)||_F^2,$$

where $N(h) = \{(\mathbf{s}_i, \mathbf{s}_j) \in D : h - \Delta h < ||\mathbf{s}_i - \mathbf{s}_j|| < h + \Delta h; i, j = 1, \ldots, n\}$, Δh is a positive (small) quantity acting as a smoothing parameter, $h > 0$ and $|N(h)|$ is the number of couples $(\mathbf{s}_i, \mathbf{s}_j)$ belonging to $N(h)$. A model semivariogram $\widehat{\gamma}_m(h)$ can be fitted to the empirical semivariogram, for example via weighted least squares. [1] advocates the use of the semivariogram to estimate the spatial dependence. However, an estimate of the covariogram is also needed and this can be obtained as $\widehat{C}(||\mathbf{s}_i - \mathbf{s}_j||) = \lim_{h\to\infty} \widehat{\gamma}_m(h) - \widehat{\gamma}_m(||\mathbf{s}_i - \mathbf{s}_j||)$. In practice a good estimate of the spatial dependence (including the choice of the model semivariogram) is crucial for the analysis. The space of symmetric matrices being linear, all the existing methods of geostatistics can be used here.

Since we aim to estimate both the spatial dependence and the linear model in the tangent space, we resort to a nested iterative algorithm to estimate the parameters of model (1). We start from initial estimates $\widehat{\Sigma}^{(0)}$ and $\widehat{\boldsymbol{\beta}}^{(0)}$ obtained by assuming independence between observations and we estimate the spatial dependence from the residuals $\widehat{\Delta}_i = A(\mathbf{x}(\mathbf{s}_i);\widehat{\boldsymbol{\beta}}^{(0)}) - \log_{\widehat{\Sigma}^{(0)}}(S_i)$, $i = 1, \ldots, n$. Then, we iteratively update the estimate for Σ and $\boldsymbol{\beta}$ taking into account the estimated covariance structure in the generalized least square procedure and revise the estimated covariance structure using the newly found residuals. The algorithm is stopped when the variation in the estimate for Σ is negligible. A detailed description of the iterative algorithm can be found in [6].

In general, this estimation procedure asks for the knowledge of the model in the tangent space. Cross-validation techniques can of course be used to choose the model among a starting set of candidate models. However, it is also important to mention that the chosen model needs tangent space residuals with a variogram compatible with stationarity. Therefore, a good strategy could be starting from a simple (even constant) model and

adding covariates until the residuals variogram satisfies the stationarity hypothesis.
Once the model has been estimated, a kriging interpolation of the residuals provides an estimate for the field S in the unobserved location $\mathbf{s}_0$. Indeed, the problem of kriging is well defined when working in the tangent space, because this is a Hilbert space with respect to the Frobenius inner product and the covariogram C has been coherently defined. It is also possible to evaluate the prediction error using a bootstrap approach (see [6] for more details).

2 Application to Quebec meteorological data

We apply the described procedure to the covariance matrices between temperature and precipitation in Quebec, Canada. The co-variability of temperature and precipitation is of great interest for meteorological purposes, since a good understanding of their relationship can improve weather forecasting methods. Moreover, relative behavior of temperature and precipitation affects agricultural production. For a detailed description of the temperature - precipitation relationship and its estimate see, e.g., [7] and references therein.
We focus on the Quebec province, Canada. Data from Canadian meteorological stations are made available by Environment Canada on the website `http://climate.weatheroffice.gc.ca`. We restrict to the 7 meteorological stations where all monthly temperature and precipitation data are available from 1983 to 1992. For each station and for each month from January to December, we use these 10-year measures to estimate the 2×2 covariance matrix between temperature and precipitation. We thus obtain and separately analyse 12 datasets, each composed by $n = 7$ spatially dependent sample covariance matrices (with the previous notation, $n = 7$ and $p = 2$).
Notice that, since we are working on different tangent spaces for the different months, a separate semivariogram needs to be estimated for each month. We discuss here the results for the month of January, a more detailed analysis can be found in [6]. At first, we make the hypothesis of stationarity for the random field (i.e., that the matrix random field has a constant mean), thus including only a constant term in the tangent space model. A Gaussian semivariogram model with nugget seems appropriate to fit the empirical semivariogram in the tangent space and estimate the structure of spatial dependence. Having estimated the semivariogram, the simple kriging interpolation of the residuals is performed, eventually estimating the matrix field. However, the semivariogram suggests to move toward a non-stationary model, by introducing a space dependent drift term.
In order to choose an appropriate model for the drift in January, we investigated linear and quadratic models with respect to longitude and latitude, including an interaction term. We found that the choice which seems to balance the most the complexity of the drift model with the residuals stationarity assumption is the following linear model depending on longitude:

$$A(\text{Longitude}_i, \text{Latitude}_i) = \beta_0 + \beta_{Long}\text{Longitude}_i. \tag{2}$$

A possible meteorological interpretation relies in the exposition of the region toward the sea. Indeed, model (2) accounts for the distance between the location of interest and the Atlantic Ocean, which is likely to influence temperatures, precipitations and their covariability.
From a meteorological point of view, the kriged map shows that the temperature - precipitation relationship appears to significantly vary when moving from the Ocean toward the internal regions, precipitation being affected by a higher variability along the

coastline than in the western zone. Moreover, this prediction is overall characterized by a positive correlation between temperature and precipitation, in accordance with the results by [7].

References

[1] Cressie, N.A.C. 1993 *Statistics for spatial data, Revised edition.* Wiley, New York.

[2] Delicado, P., Giraldo, R., Comas, C. and Mateu, J. 2010 *Statistics for spatial functional data: some recent contributions.* Environmetrics, 21, 224–239.

[3] Fletcher, P.T. 2013 *Geodesic Regression and the Theory of Least Squares on Riemannian Manifolds.* Int. J. Comput. Vision. 2, 171–185.

[4] Gromenko, O., Kokoszka, P., Zhu, L. and Sojka, J. 2012 *Estimation and testing for spatially indexed curves with application to ionospheric and magnetic field trends.* Ann. Appl. Stat. 6, 669–696.

[5] Menafoglio, A., and Petris, G. 2015 *Kriging for Hilbert-space valued random fields: the Operatorial point of view.* J. Multivariate Anal. 146, 84–94.

[6] Pigoli, D., Menafoglio, A. and Secchi, P. 2016 *Kriging prediction for manifold-valued random fields.* J. Multivariate Anal. 145, 117–131.

[7] Trenberth, K.E. and Shea, D.J. 2005 *Relationship between precipitation and surface temperature.* Geophys. Res. Lett. 32, L14703.

Mathematical-Physical Models for Dynamic and Thermodynamic Processes - Part I

PROPOSERS

Liliana Restuccia
Universitá di Messina
Viale F. Stagno d'Alcontres, 31 98166 - Messina Italy
lrestuccia@unime.it

David Jou
Universitat Autònoma de Barcelona
08193 - Bellaterra Spain
david.jou@uab.cat

Maria Stella Mongioví
Universitá di Palermo
Viale delle Scienze 90128 - Palermo Italy
m.stella.mongiovi@unipa.it

Michele Sciacca
Universitá di Palermo
Viale delle Scienze 90128 - Palermo Italy
michele.sciacca@unipa.it

SPEAKERS

David Jou
Departament de Física, Universitat Autònoma de Barcelona
david.jou@uab.cat

Liliana Restuccia
Dipartimento di Scienze Matematiche ed Informatiche, Scienze Fisiche e Scienze della Terra, Università di Messina,
lrestuccia@unime.it

Michele Sciacca
Dipartimento di Scienze Agrarie e Forestali, Universitá di Palermo
michele.sciacca@unipa.it

F. Xavier Alvarez
Departament de Física, Universitat Autònoma de Barcelona
xavier.alvarez@uab.cat

Lidia Saluto
DEIM, Universitá degli studi di Palermo
lidia.saluto@unipa.it

This Minisymposium is devoted to discuss the last researches on the following topics:

- Description of dynamic and thermodynamic processes in material systems studied in several fields of applied sciences: nanostructures, semiconductors, superfluids, ionized fluids, crystals with dislocations, porous media, biophysical systems, complex media;
- Derivation of constitutive equations and heat transport equation in thermodynamic systems, used in several technologic sectors;
- Realization of physical-mathematical models used to illustrate phenomena occurring in different fields of science.

The participation in this Minisymposium will allow researchers of Mathematical-Physics to deepen research subjects, to know several open problems and new methods of investigation, to realize scientific contacts with italian and foreign mathematical-physicists.

Non-equilibrium entropies and non-linear viscoelasticity

David Jou
Universitat Autònoma de Barcelona
Departament de Física, Edifici Cc, 08193 Bellaterra, Catalonia, Spain
david.jou@uab.cat

Mengram Sun
National Engineering Laboratory for Pipeline Safety,
China University of Petroleum, Beijing 102249 China

It is shown that if instead of the fluxes, their conjugate thermodynamic quantities -as defined in extended irreversible thermodynamics [1]- are used as independent variables of the entropy, a generalized equation for non-linear viscoelasticity arises in a natural way [2, 3]. Such equation takes into account the structure dependence of the elastic modulus and of the viscosity, and it was proposed independently several years ago [4]. Finally, we point the advantages of this equation with respect to Maxwell viscoelastic equation in the description of yielding of waxy crude oils [2].

References

[1] D. Jou, J. Casas-Vázquez and G. Lebon, *Thermodynamics of fluids under flow*, Springer, Berlin, 2011

[2] M. Sun, D. Jou, J. Zhang, *A non-linear viscoelastic model and non-equilibrium entropies*, Journal of Non-Newtonian Fluid Mechanics 229 (2016) 96-100

[3] Y. Zhu, L. Hong, Z. Yang, W. Yong, *Conservation-dissipation formalism for irreversible thermodynamics*, J. Non-Equilib. Thermodyn. 40 (2015) 67-74

[4] G. Marrucci, G. Titomanlio, G. C. Sarti, *Testing of a constitutive equation for entangled networks by elongational and shear data of polymer melts*, Rheol. Acta 12 (1973) 269-275

Non equilibrium processes and heat equation in defective extrinsic semiconductors

Liliana Restuccia
Università degli Studi di Messina
Viale F. S. D' Alcontres 31, 98166, Messina, Italy
lrestuccia@unime.it

David Jou
Universitat Autònoma de Barcelona
08193 Bellaterra, Catalonia, Spain
David.Jou@uab.cat

In this contribution, in the framework of the extended irreversible thermodynamics with internal variables [1],[2],[3],[4], a nonconventional model for extrinsic semiconductor crystals with dislocations, derived in a previous paper [5], by one of the authors (LR), is used in order to study the thermal, electric, mechanical properties and the evolution of the geometrical structure of these materials and to analyze the influence of the defects on the non-equilibrium processes that occur inside them. In the linear approximation, constitutive equations, rate equations for the heat flux and the internal variables are derived and also the field equations are worked out. The obtained results may have relevance in nanotechnology, in applied computer science, in the technology for integrated circuits VLSI (Very Large Scale Integration), in the field of electronic microscopy and in other technological sectors.

References

[1] Jou, D., Casas-Vazquez, J. and Lebon, G. 2010 *Extended Irreversible Thermodynamics.* Springer, Berlin, fourth ed.

[2] Lebon, G., Casas-Vazquez, J., and Jou, D. 2008 *Understanding Non-Equilibrium Thermodynamics.* Springer, Berlin.

[3] Jou, D. and Restuccia, L. 2011 *Mesoscopic transport equations and contemporary thermodynamics: an introduction.* Contemporary Physics 52 (5), 465-474.

[4] Muschik, W. 1993 *Non-Equilibrium Thermodynamics with Applications to Solids*, 336, Springer, Wien-New York.

[5] Restuccia, L. and Maruszewski, B. 1995 *Interactions between electronic field and dislocations in a deformable semiconductor.* Int. J. Applied Electromagnetics and Mechanics, 6, 139-153.

A mathematical model to describe the glitches in rotating superfluids

Michele Sciacca
Università degli Studi di Palermo
viale delle Scienze, Ed. 4 90128 - Palermo Italy
michele.sciacca@unipa.it

Maria Stella Mongiovì
Universitá degli Studi di Palermo
viale delle Scienze, Ed. 8 90128 - Palermo Italy
m.stella.mongiovi@unipa.it

Francesco Russo
University of Cape Town
Private Bag X1, 7701, Rondebosch, Cape Town South Africa
francescog.russo@yahoo.com

The complete knowledge of glitches in a pulsar presents gaps and difficulties, mainly due to the absence of information about the physics of the matter of the star. This motivated several authors to suggest dynamical models, which interpret most of the experimental data [1, 2, 3, 4, 5, 6]. Many predictions are based on the assumption that the inner part has analogies with the structure of the matter of superfluids [7]. Here we illustrate a new mathematical model, which involves the dynamics of superfluid helium. More in details, we consider the system [8]

$$\begin{cases} I_C \frac{d\Omega_C}{dt} = -k_r^C - \frac{1}{\tau}\frac{I_S I_C}{I_S+I_C}\left(\Omega_C - \frac{\kappa L}{2}\right) \\ I_S \frac{d\Omega_S}{dt} = -k_r^S + \frac{1}{\tau}\frac{I_S I_C}{I_S+I_C}\left(\Omega_C - \frac{\kappa L}{2}\right) \\ \frac{1}{\beta\kappa}\frac{dL}{dt} = -\left(L - \frac{2\Omega_S}{\kappa}\right)\left[L - \left(\frac{\alpha_1}{\beta}\frac{\Omega_{SC}}{\kappa} - \frac{\beta_1}{\beta}\frac{\Omega_S}{\kappa}\right)\right]. \end{cases} \tag{1}$$

where $k_r = k_r^C + k_r^S$ is the total torque due to the electromagnetic radiation. The first two evolution equations for the angular velocities of the crust, Ω_C, and of the inner part, Ω_S, are supported by another evolution equation for the average vortex line length per unit volume, L.
We claim that the phenomena of glitch is caused by quantized vortex lines, which are present inside the superfluid neutron liquid, and by means of the relative velocity between the crust and the inner part of the neutron star. Indeed, in the first regime (straight vortex regime) crust and inner part of the star corotate in such a way that vortex lines are straight lines parallel to the rotation axis and pinned to the crust. Because of the slowing down of the crust, the relative velocity (between crust and superfluid) increases and reaches a critical value for the unpinning of the vortex lines. This transient is described by the parameter of time, τ, and here we find a sudden increase of the velocity of the crust and so the glicth. Our model is also applied to the experiments on rotating superfluid

helium inside a sphere [7] for future applications in refrigeration of systems or in aerospace technology.

References

[1] Anderson, N., Comer, G.L. and Sidery T. 2007 *Superfluid neutron star turbulence*. Mon. Not. R. Astron. Soc. 381, 747–756.

[2] Baghdasaryan, D., Hayrapetyan, M. V. and Sedrakian, D. M. 2014 *Relaxation of the Angular Velocity of Pulsars after Glitches*. Astroph. 57, 90–104.

[3] Chukwude, A.E., Joshi, B.C. and Urama, J.O. 2013 *On the Glitch Evolution of Pulsars*. Proc. Int. Astron. Union 291, 533–535.

[4] Fattoyev, F. J. and Piekarewicz, J. 2010 *Sensitivity of the Moment of Inertia of Neutron Stars to the Equation of State of Neutron-Rich Matter*. Phys. Rev. C 82.

[5] Packard, R.E. 1972 *Pulsar speedups related to metastability of the superfluid neutron-star core*. Phys. Rev. Lett. 28, 1080–1082.

[6] Padmanabhan, T. 2001 *Theoretical Astrophysics, Vol. II: Stars and Stellar Systems*, Cambridge University Press, Cambridge.

[7] Tsakadze, J.S. and Tsakadze, S.J. 1980 *Properties of slowly rotating helium II and the superfluidity of pulsars*. J. Low Temp. Phys. 39, 649–688.

[8] Mongioví, M.S., Russo, F. and Sciacca, M. 2016 *A mathematical description of glitches in neutron stars* (under review).

Kinetic Collective Model and the microscopic foundation of phonon hydrodynamics

F. Xavier Alvarez
Universitat Autònoma de Barcelona
Departament de Física, Edifici Cc, 08193 Bellaterra, Catalonia, Spain
xavier.alvarez@uab.cat

Pol Torres
Universitat Autònoma de Barcelona
Departament de Física, Edifici Cc, 08193 Bellaterra, Catalonia, Spain
pol.torres@uab.cat

Xavier Cartoixà
Universitat Autònoma de Barcelona
Departament d'Enginyeria, Edifici Q, 08193 Bellaterra, Catalonia, Spain
xavier.cartoixa@uab,cat

Javier Bafaluy
Universitat Autònoma de Barcelona
Departament de Física, Edifici Cc, 08193 Bellaterra, Catalonia, Spain
javier.bafaluy@uab,cat

Juan Camacho
Universitat Autònoma de Barcelona
Departament de Física, Edifici Cc, 08193 Bellaterra, Catalonia, Spain
juan.camacho@uab,cat

Àlvar Torelló
Universitat Autònoma de Barcelona
Departament de Física, Edifici Cc, 08193 Bellaterra, Catalonia, Spain

Recent experiments in heat transport on silicon using ultrafast laser heating techniques have shown significant discrepancies with Fourier like behaviour. [1, 2, 3, 4]. The interpretations of these results using only a ballistic to diffusive transition of the carriers have shown to be unfruitful. The reason behind this anomalous behaviour seems to be momentum conserving collisions (normal scattering). In materials like silicon, normal scattering can be dominant at room temperature. When this kind of collisions are dominant, collective (hydrodynamic) effects are important.
Kinetic-Collective Model (KCM) is an approach that has been recently proposed to describe thermal transport at these time and size scales [5, 6]. The model splits the heat flux in two regimes, a kinetic one where each carrier is independent of the rest and a collective where they move collectively. Kinetic and collective regimes behave very differently at short scales. While kinetic regime follows a Levy Flights like transport [7], collective regime shows hydrodynamic behaviour[8].

We use KCM to interpret the recent experimental results and show that some of their complexities can be understood in the light of a kinetic to collective transition.

References

[1] M. E. Siemens, Q. Li, R. Yang, K. A. Nelson, E. H. Anderson, M. M. Murnane, and H. C. Kapteyn, "Quasi-ballistic thermal transport from nanoscale interfaces observed using ultrafast coherent soft X-ray beams," *Nature Materials*, vol. 9, no. 1, pp. 26–30, 2010.

[2] J. A. Johnson, A. A. Maznev, J. Cuffe, J. K. Eliason, A. J. Minnich, T. Kehoe, C. M. S. Torres, G. Chen, and K. A. Nelson, "Direct Measurement of Room-Temperature Nondiffusive Thermal Transport Over Micron Distances in a Silicon Membrane," *Physical Review Letters*, vol. 110, p. 025901, jan 2013.

[3] R. B. Wilson and D. G. Cahill, "Anisotropic failure of Fourier theory in time-domain thermoreflectance experiments.," *Nature communications*, vol. 5, p. 5075, jan 2014.

[4] K. M. Hoogeboom-Pot, J. N. Hernandez-Charpak, X. Gu, T. D. Frazer, E. H. Anderson, W. Chao, R. W. Falcone, R. Yang, M. M. Murnane, H. C. Kapteyn, and D. Nardi, "A new regime of nanoscale thermal transport: Collective diffusion increases dissipation efficiency," *Proceedings of the National Academy of Sciences*, vol. 112, p. 201503449, mar 2015.

[5] C. D. Tomas, A. Cantarero, and F. X. Alvarez, "Phonon-phonon interactions of group-IV semiconductors: Predicting Thermal conductivity," no. 5, pp. 1–6, 2014.

[6] C. D. Tomas, A. F. Lopeandia, F. X. Alvarez, and A. Cantarero, "From kinetic to collective behavior in thermal transport on semiconductors and semiconductor nanostructures: The limit of classical theories.," 2014.

[7] B. Vermeersch, J. Carrete, N. Mingo, and A. Shakouri, "Superdiffusive heat conduction in semiconductor alloys – I. Theoretical foundations," pp. 1–10, jun 2014.

[8] A. Sellitto, F. Alvarez, and D. Jou, "Geometrical dependence of thermal conductivity in elliptical and rectangular nanowires," *International Journal of Heat and Mass Transfer*, vol. 55, pp. 3114–3120, may 2012.

Heat flux in He II in inhomogeneous channels

Lidia Saluto
Istituto di Alta Matematica "F. Severi" (GNFM)
lidia.saluto@unipa.it

Maria Stella Mongiovì
Università degli Studi di Palermo
Viale delle Scienze, 90128 - Palermo Italy
m.stella.mongiovi@unipa.it

David Jou
Universitat Autònoma de Barcelona
08193 - Bellaterra Spain
david.jou@uab.cat

One of the most typical effects in liquid helium II is the so-called *counterflow superfluid turbulence* [1, 2, 3], whose physical picture is a tangle of vortices of equal circulation κ. The simplest way to describe the vortex tangle is in terms of a single scalar quantity L, the vortex length density per unit volume (line density, for short). Vinen, first, proposed an evolution equation for L under constant counterflow velocity $V_{ns} = |\mathbf{v}_n - \mathbf{v}_s|$, with $\mathbf{v}_n$ and $\mathbf{v}_s$ the average velocities of normal and superfluid components, i.e. [4] :

$$\frac{dL}{dt} = \alpha_v V_{ns} L^{3/2} - \beta_v \kappa L^2, \tag{1}$$

with α_v and β_v dimensionless parameters. The quantity $\mathbf{V}_{ns}$ is closely related to the heat flux $\mathbf{q}$ (in the simplest version, $\mathbf{q} = \rho_s T s \mathbf{V}_{ns}$, with T temperature, ρ_s mass density of the superfluid component and s entropy per unit mass). This equation assumes homogeneous turbulence, i.e. that the value of L is the same everywhere in the system.
The progress in experiments and computations has allowed for deeper observation, which shows that the tangles are not completely homogeneous. Our aim here is to study some particular situations, as the vortex diffusion, in specific geometries that present inhomogeneous vortex tangles. We will use the one-fluid model deduced from extended thermodynamics [5], assuming as field variables T, L, and $\mathbf{q}$. In particular we will consider for L a generalized Vinen equation:

$$\frac{\partial L}{\partial t} = \gamma_1 L^{3/2} q - \beta_v \kappa L^2 + D \nabla^2 L - \nu \nabla \cdot \mathbf{q}. \tag{2}$$

The first two terms, respectively, describe production and destruction of vortices and are analogous to the right-hand side of (1); term $D\nabla^2 L$ takes into account of diffusive phenomena, while the term $-\nu \nabla \cdot \mathbf{q}$ relates a convective flux of vortices to the heat flux. In [6] we considered the consequence of (2) in a radial geometry [6], here we consider convergent and divergent channels of different forms and analyze the L and T profiles along the channels for a given direct and reverse heat flux, and the subsequent heat rectification effects.

References

[1] Donnelly R.J., Quantized vortices in helium II. Cambridge University Press, Cambridge 1991.

[2] C.F. Barenghi, R.J. Donnelly and W.F. Vinen, Quantized Vortex Dynamics and Superfluid, Turbulence. Springer, Berlin 2001.

[3] Nemirovskii S.K., Quantum turbulence: Theoretical and numerical problems. Physics Reports 524.3 (2013): 85-202.

[4] Vinen W.F., Mutual friction in a heat current in liquid helium II. III. Theory of the mutual friction. Proc. Royal Society of London A. Vol. 242. No. 1231. 1957.

[5] Mongiovì M.S. and D. Jou, Thermodynamical derivation of a hydrodynamical model of inhomogeneous superfluid turbulence, Phys. Rev. B, 75 (2007), 024507.

[6] Saluto L., Jou D., and Mongiovì M.S., Vortex diffusion and vortex-line hysteresis in radial quantum turbulence. Physica B 440 (2014): 99-103.

Mathematical-Physical Models for Dynamic and Thermodynamic Processes - Part II

PROPOSERS

Liliana Restuccia
Universitá di Messina
Viale F. Stagno d'Alcontres, 31 98166 - Messina Italy
lrestuccia@unime.it

David Jou
Universitat Autònoma de Barcelona
08193 - Bellaterra Spain
david.jou@uab.cat

Maria Stella Mongioví
Universitá di Palermo
Viale delle Scienze 90128 - Palermo Italy
m.stella.mongiovi@unipa.it

Michele Sciacca
Universitá di Palermo
Viale delle Scienze 90128 - Palermo Italy
michele.sciacca@unipa.it

SPEAKERS

Orazio Muscato
Dipartimento di Matematica e Informatica, Universitá di Catania
muscato@dmi.unict.it

Antonio Sellitto
Dipartimento di Ingegneria Industriale, Universitá di Salerno
asellitto@unisa.it

This Minisymposium is devoted to discuss the last researches on the following topics:

- Description of dynamic and thermodynamic processes in material systems studied in several fields of applied sciences: nanostructures, semiconductors, superfluids, ionized fluids, crystals with dislocations, porous media, biophysical systems, complex media;
- Derivation of constitutive equations and heat transport equation in thermodynamic systems, used in several technologic sectors;
- Realization of physical-mathematical models used to illustrate phenomena occurring in different fields of science.

The participation in this Minisymposium will allow researchers of Mathematical-Physics to deepen research subjects, to know several open problems and new methods of investigation, to realize scientific contacts with italian and foreign mathematical-physicists.

A quantum-kinetic approach to describe transport phenomena in semiconductors

Orazio Muscato
Dipartimento di Matematica e Informatica, Università degli Studi di Catania
viale A. Doria, 6 95125 - Catania Italy
muscato@dmi.unict.it

Coherent transport in mesoscopic devices is well described by the Schrödinger equation supplemented by open boundary conditions. When electronic devices are operated at room temperature, however, a realistic transport model needs to include carrier scattering. The Wigner formulation of quantum mechanics is a very intuitive approach which allows the comprehension and prediction of quantum mechanical phenomena in terms of quasi distribution functions. Carrier scattering can be treated in an approximate manner through a Boltzmann collision operator. A Monte Carlo technique for the solution of this kinetic equation can been developed, based on an interpretation of the Wigner potential.

References

[1] O. Muscato and W. Wagner, *A class of stochastic algorithms for the Wigner equation*, to appear in *SIAM Journal on Scientific Computing*

Nonlinear heat-transport equation beyond Fourier law: Application to heat-wave propagation in isotropic thin layers

Antonio Sellitto
University of Salerno
Campus of Fisciano, 84084, Fisciano, Italy
asellitto@unisa.it

Vincenzo Tibullo
University of Salerno
Campus of Fisciano, 84084, Fisciano, Italy
vtibullo@unisa.it

Yuan Dong
University of Missouri
Columbia, Missouri, 65211, USA
dony327@163.com

Since the last decades of the XXth century, heat transport has been experiencing a true revolution, enlarging its domain of applicability, and finding new regimes and phenomenologies wherein Fourier's theory is no longer applicable. This new epoch in heat transfer has been stimulated by nanotechnologies which have an extremely broad range of potential applications.
Much of the impetus in the study of heat transfer in nanostructures and/or nanomaterials comes from microscopic approaches, either from several versions of kinetic theory or fluctuation-dissipation theorems, or from computer simulations. Although these approaches allow for a detailed understanding and description, one should not forget the practical usefulness and the conceptual challenge of mesoscopic theories which, starting from macroscopic perspectives, deepen into more detailed and accurate descriptions of those thermomechanical systems.
According with this point of view, in this talk we investigate the consequences on thermal-wave propagation of a generalized heat-transport law able to keep with the pace of current microscopic search, and to cope efficiently with new applications [1].
In order to analyze situations which may be interesting in practical applications, we focus our attention in thin layers and graphene stripes which are not laterally isolated from the external environment.
A comparison with the approach of the Thermomass Theory [2, 3] is made as well.

References

[1] Sellitto, A. and Cimmelli, V. A. and Jou, D. 2016 *Mesoscopic Theories of Heat Transport in Nanosystems.* Springer International Publishing.

[2] Dong, Y. and Cao, B.-Y. and Guo, Z.-Y. 2011 *Generalized heat conduction laws based on thermomass theory and phonon hydrodynamics.* J. Appl. Phys. 110, 063504 (6 pages).

[3] Sellitto, A. and Cimmelli, V. A. 2012 *A continuum approach to thermomass theory.* J. Heat Trans. -– T. ASME 134, 112402 (8 pages).

Mathematical techniques for geological basin modelling

PROPOSERS

Matilde Dalla Rosa
Eni S.p.A. Upstream and Technical Services
via Emilia, 1 20097 - san Donato Milanese, Milan, Italy
matilde.dalla.rosa@eni.com

Anna Scotti
Politecnico di Milano
Pzza Leonardo da Vinci, 32 20133 - Milano Italy
anna.scotti@polimi.it

SPEAKERS

Fabio Vicini
Dept. Mathematics, Politecnico di Torino
fabio.vicini@polito.it

Daniele Rossi
Dept. of Mathematics, Politecnico di Milano
niredda@gmail.com

Giulia Ceriotti
DICA - Dept. of Civil and Environmental Engeneering, Politecnico di Milano
giulia.ceriotti@polimi.it

Alfredo Battistelli
SAIPEM, AMBEN Dept. / Reservoir Modelling and Engineering
alfredo.battistelli@saipem.com

Hydrocarbon exploration is a complex activity, based on a high level geological and geophysical competence, and consolidated processes including seismic imaging, the modelling of petroleum systems and cutting-edge drilling.
The appropriate application of these technologies enables to explore new areas generally characterized by very complex geological and environmental conditions. Being able to describe the subsoil and to estimate the amount and quality of fluids contained in sedimentary reservoirs is crucial to reduce exploration risk, and oil industry is resorting more and more often to mathematical modeling and numerical simulations to this purpose. This minisymposium aims at collecting contributions on mathematical models, tools, software and workflows for exploration, focusing in particular on geological basin modelling and fluid flow.

References

[1] Giovanardi, B., Scotti, Formaggia, L., A., Ruffo, P., *A general framework for the simulation of geochemical compaction*, Computational Geosciences 19(5) (2015).

[2] Cathles, L., Schoell, M. 2007. *Modeling CO2 generation, migration, and titration in sedimentary basins.* Geofluids, 7(4), 441-450.

[3] Pruess K., Battistelli A. 2002. *TMVOC, a numerical simulator for three-phase non-isothermal flows of multicomponent hydrocarbon mixtures in saturated-unsaturated heterogeneous media.* LBNL-Report 49375, Lawrence Berkeley National Laboratory, Berkeley, CA.

GEOSCORE-Flow, a flexible C++ parallel code for flow simulation in fractured media: mixing discretization approaches and solvers

Fabio Vicini
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
fabio.vicini@polito.it

Stefano Berrone
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
stefano.berrone@polito.it

Andrea Borio
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
andrea.borio@polito.it

Sandra Pieraccini
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
sandra.pieraccini@polito.it

Stefano Scialò
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
stefano.scialo@polito.it

We focus on the issue of performing efficient flow simulations in fractured media following the Discrete Fracture Network (DFN) framework. Within this approach, the medium is modelled as a rock matrix crossed by a net of polygonal fractures. Fractures do intersect each other along segments called *traces*. The flow on each fracture is driven by the Darcy law, the rock matrix is impervious so that there is not flux exchange between the fracture system and the surrounding rock, but there is flux exchange among fractures through their intersection. At fractures intersections, suitable matching conditions are imposed, ensuring hydraulic head continuity and flux balance. Since few deterministic information is available about the underground, the DFNs are usually generated starting from known probabilistic distributions both for hydro-geological and geometrical parameters. Concerning the latter ones, they include position, dimensions, aspect ratio and orientation in space. As a consequence, the network generated may present a rather complex geometry, with several critical features, such as, for example, trace length with a multi-scale distribution, traces on a same fracture forming very narrow angles, and so on. In Figure 1 an example of large, complex DFN is depicted.

These geometrical complexities may cause severe problems in building a good quality

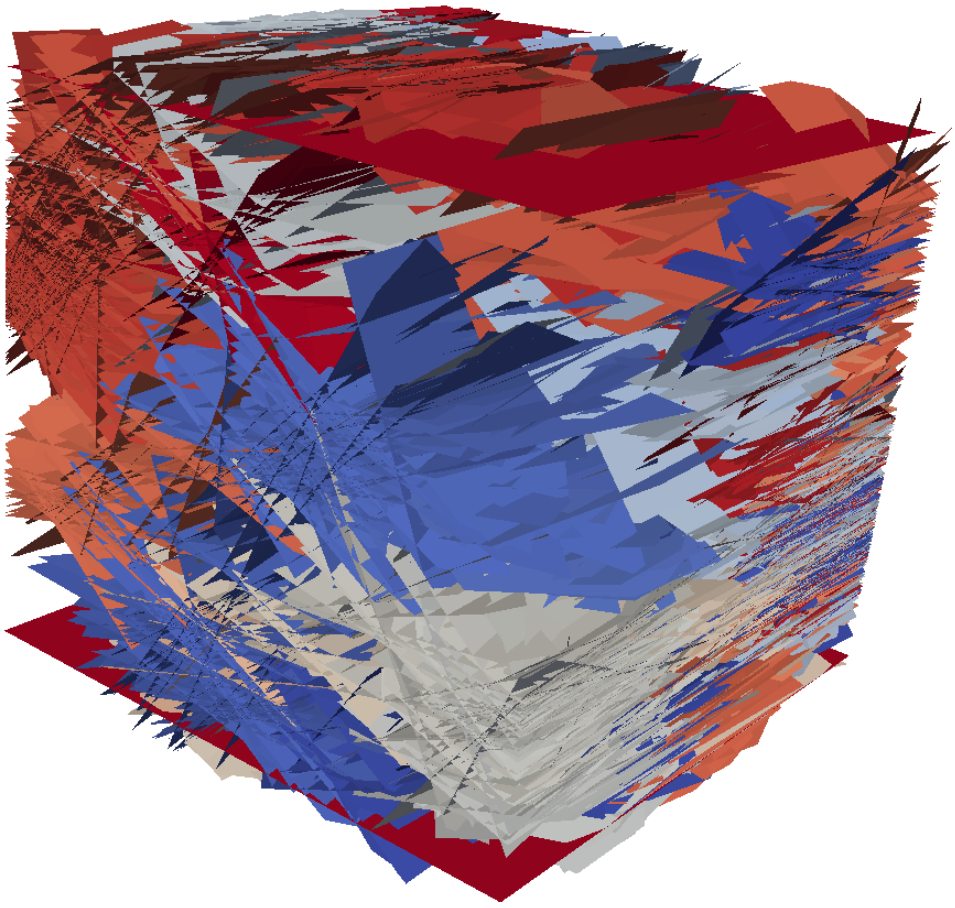


Figure 1: An example of network

mesh conforming to the traces. A new optimization based approach was proposed in [4, 5, 6], allowing for non-conforming meshes on the fractures, thus avoiding any mesh related complexity in DFN flow simulations. The optimization method has proven to be robust with respect to severe geometrical configurations [8, 7]. Besides geometrical complexity, a second major challenge in DFN simulations is related to the size of the computational domain. Networks of interest for practical applications might count up to several thousands of fractures, such that a strongly parallel method with an efficient handling of computational resources is mandatory.

The present contribution focuses on the parallel implementation of the family of methods generated by [4] and following papers. According to the reformulation proposed in such works, the discrete problem one has to solve consists in a quadratic programming problem with linear equality constraints, which is iteratively solved by means of a gradient based method. At each iteration of the gradient method only small local problems on the fractures are to be solved, the resolution of each problem requiring data on the trace segments of the intersecting fractures. The parallel implementation of the method exploits this structure. First the connectivity of the network is computed, determining intersections between fractures in a parallel process, in which the total number of operations is balanced among the number of available processes. The output is a connected graph, in which the fractures are the nodes and the traces the arcs, Figure 2. The METIS [10] routine is then used to compute a weighted graph partitioning of the network, aimed at minimizing

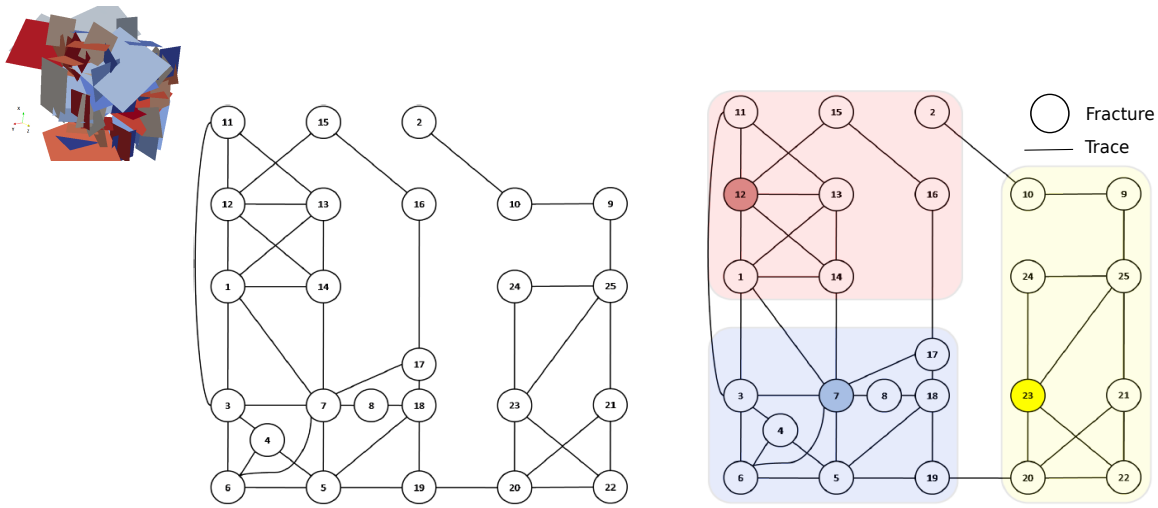


Figure 2: Balanced Graph partitioning process

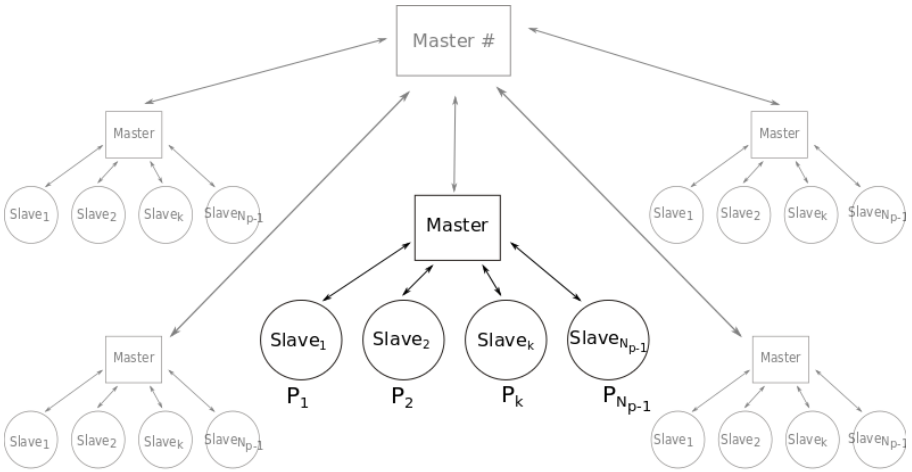


Figure 3: (Multi)-Master/Slave architecture

the number of arc-cuts, balancing the estimated number of degrees of freedom (DOFs) among the sub-graphs. The DFN is then split a second time according to this partitioning among the available processes. A Master-Slaves architecture is the core topology devised for the algorithm: a Master process is devoted to all the communications among the Slave processes that are instead devoted to the computations. This topology minimizes the number of communications, thus reducing latency time. A multi Master architecture can also be used in order to reduce the possible communication bottleneck for large networks. In this case the basic Master-Slave topology is repeated in a fractal-like structure, with higher level Master processes managing the communications of clusters of lower level Master processes, down to the Slave processes, see Figure 3. The bandwidth is extremely limited in this kind of applications, since as mentioned, only a limited number of degrees of freedom, related to the solution on the traces need to be communicated at each iteration. Particular care is devoted to shadowing the communication time, postponing, on each process, the resolution of local problems related to data resident on different processes to the resolution of local problems whose data are all available. This latter situation is not

uncommon, thanks to the minimization of arc-cuts in the partitioning process. Thanks to this good scalability performances can be achieved [8]. The algorithm is written in `C++` language, with a focus on modularity: different discretization starategies, such as standard Finite Elements or eXtended Finite Elements (XFEM) [9] can be used as a basis for the discretization. Other techniques such as the Virtual Elements (VEM) [1] based discretizations can be considered such as other resolution approaches different from the gradient based method, as for example domain decomposition methods in conjunction with VEM-mortar approaches [2] or VEM-conforming approaches [3].

References

[1] L. Beirão da Veiga, F. Brezzi, A. Cangiani, G. Manzini, L. D. Marini, and A. Russo. Basic principles of virtual element methods. *Mathematical Models and Methods in Applied Sciences*, 23(01):199–214, 2013.

[2] M.F. Benedetto, S. Berrone, A. Borio, S. Pieraccini, and S. Scialò. A Hybrid Mortar Virtual Element Method For Discrete Fracture Network Simulations. *J. Comput. Phys.*, 306:148–166, 2016.

[3] M.F. Benedetto, S. Berrone, and S. Scialò. A Globally Conforming Method For Solving Flow in Discrete Fracture Networks Using the Virtual Element Method. *Finite Elem. Anal. Des.*, 109:23–36, 2016.

[4] S. Berrone, S. Pieraccini, and S. Scialò. A PDE-constrained optimization formulation for discrete fracture network flows. *SIAM J. Sci. Comput.*, 35(2):B487–B510, 2013.

[5] S. Berrone, S. Pieraccini, and S. Scialò. On simulations of discrete fracture network flows with an optimization-based extended finite element method. *SIAM J. Sci. Comput.*, 35(2):A908–A935, 2013.

[6] S. Berrone, S. Pieraccini, and S. Scialò. An optimization approach for large scale simulations of discrete fracture network flows. *J. Comput. Phys.*, 256:838–853, 2014.

[7] S. Berrone, S. Pieraccini, and S. Scialò. Towards effective flow simulations in realistic discrete fracture networks. *J. Comput. Phys.*, 310:181–201, 2016.

[8] S. Berrone, S. Pieraccini, S. Scialò, and F. Vicini. A parallel solver for large scale DFN flow simulations. *SIAM J. Sci. Comput.*, 37(3):C285–C306, 2015.

[9] Thomas-Peter Fries and Ted Belytschko. The extended/generalized finite element method: an overview of the method and its applications. *Internat. J. Numer. Methods Engrg.*, 84(3):253–304, 2010.

[10] G. Karypis and V. Kumar, A fast and high quality multilevel scheme for partitioning irregular graphs. *SIAM Journal on Scientific Computing*, 20:359–392, 1998.

Numerical simulation of hydrocarbons generation in the source rock

Daniele Rossi
Dipartimento di Matematica, Politecnico di Milano
piazza Leonardo da Vinci 32, 20133 - Milano Italy
niredda@gmail.com

Matilde Dalla Rosa
Eni S.p.A. Upstream and Technical Services
via Emilia, 1 20097
san Donato Milanese - Milano Italy matilde.dalla.rosa@eni.com

Anna Scotti
Dipartimento di Matematica, Politecnico di Milano
piazza Leonardo da Vinci 32, 20133 - Milano Italy
anna.scotti@polimi.it

Luca Bonaventura
Dipartimento di Matematica, Politecnico di Milano
piazza Leonardo da Vinci 32, 20133 - Milano Italy
luca.bonaventura@polimi.it

The present work focuses on generation and primary migration of hydrocarbons, with the aim of developing a mathematical model of these processes, and an efficient numerical tool to simulate them. Given the thermal history of the basin, the physical characteristics of the source rock such as porosity and organic matter content, and a detailed enough description of chemical reactions and retention processes, the model could provide, in addition to an estimate of the amount of hydrocarbons generated throughout hundreds of million years, indications on the timing of expulsion and the chemical composition of the expelled hydrocarbon. Since secondary migration is typically very fast compared to primary migration, knowing the time of expulsion allows to check for the existence of a possible trap for the generated hydrocarbons, and thus to infer the existence of a reservoir, supporting the reconstructions made by the geologists.
The problem is characterized by a strong coupling among chemical reactions, which may include biological processes [2], selective retention phenomena and the flow of water and hydrocarbons in the porosity of the rock. Porosity changes affect the flow through the medium permeability and fluid pressure can counteract mechanical compaction. At the same time, chemical reactions can cause dramatic changes in the porosity, [1].
The numerical challenges in the simulation of these processes are multiple. The most prominent ones are the definition of a coupled non-linear system that should be solved with a suitable iterative method [3], the compliance with mass conservation up to some desired tolerance, the evolution of the domain due to the compaction of the medium, the formation/dissolution of the solid matrix, the different time scales involved.

References

[1] A. Agosti, L. Formaggia, A. Scotti, Analysis of a model for precipitation and dissolution coupled with a darcy flux, Journal of Mathematical Analysis and Applications doi:10.1016/j.jmaa.2015.06.003.

[2] M. Cokar. *Biogenic Methane Generation in Shallow Shale Gas Systems, PhD thesis.* 2013.

[3] B. Giovanardi, A. Scotti, L. Formaggia, P. Ruffo, A general framework for the simulation of geochemical compaction, Computational Geosciencesdoi:10.1007/s10596-015-9518-3.

Modeling Non-Hydrocarbon Components In Sedimentary Basins

Giulia Ceriotti
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
giulia.ceriotti@polimi.it

Giovanni Michele Porta
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
giovanni.porta@polimi.it

Claudio Geloni
Eni S.p.A.-Upstream and Technical Services
via Emilia, 1 20097 San Donato Milanese (MI) Italy
claudio.geloni@eni.com

Matilde Dalla Rosa
Eni S.p.A.-Upstream and Technical Services
via Emilia, 1 20097 San Donato Milanese (MI) Italy
matilde.dalla.rosa@eni.com

Alberto Guadagnini
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
alberto.guadagnini@polimi.it

We investigate the contribution of a variety of inorganic geochemical and physical processes to the generation of CO_2 and non-hydrocarbon components, such as H_2S, in sedimentary basins. The most relevant mechanisms of CO_2 generation from inorganic sources include (*a*) Magma Degassing (MD), (*b*) Carbonate/Clay Reactions (CCR), and (*c*) Thermal Decomposition of Carbonates (TDC). Otherwise, subsurface generation of H_2S gas is mainly associated with Thermal Sulphate Reduction (TSR) processes. Since CO_2 released by magma degassing is often treated as a purely random component, we do not include it in our modeling effort. Each mechanism considered in this study plays an active role in the generation process according to specific local mineralogy and temperature/pressure conditions. We develop a physically-based mathematical formulation which enables us to characterize the main features of non-hydrocarbon component generating processes and estimate the amounts of non-hydrocarbon components generated in large scale subsurface systems. Our approach is grounded on two coupled sub-models: (*i*) a one-dimensional compaction model, providing the dynamic evolution of porosity, temperature and pressure along the vertical direction [3], and (*ii*) a chemical model, characterizing the set of relevant chemical reactions describing the way the interaction between mineral phases and pore-water may vary with depth for each of the

considered processes (see [1] and [2]). As a test bed, we analyze a suite of case studies which are representative of realistic sedimentary settings. Our model allows (*i*) identifying the contribution of the mechanisms analyzed in a given basin; (*ii*) estimating the depth at which the source of non-hydrocarbon components is located; and (*iii*) quantifying the amount of non-hydrocarbon components generated, on the basis of the mineralogy of the sediments involved in the basin formation process. We then quantify the way parameter uncertainty is propagated to model outputs by focusing on CO_2 generation through CCR, the activation of which is associated with lower temperatures than TDC. We do so by performing a global sensitivity study of the quantity of generated CO_2, as driven by uncertain chemical equilibrium constants. These are considered as key sources of uncertainty in our modeling approach because temperature and pressure distributions associated with deep burial depths typically fall outside the range of validity of commonly employed geochemical datasets. Finally, we analyze the impact of the mineralogy of the sediments on the activation of CCR processes. Our results are conducive to a critical assessment of the relevance of CCR in the generation of CO_2 under realistic field conditions.

References

[1] Cathles, L. and Schoell, M. 2007 *Modeling CO2 generation, migration, and titration in sedimentary basins.* Geofluids 7(4), 441–450.

[2] Coudrain-Ribstein, A., Gouze, P. and de Marsily, G. 1998 *Temperature-carbon dioxide partialpressure trends in confined aquifers.* Chemical Geology 145(1), 73–89.

[3] Formaggia, L., Guadagnini, A., Imperiali, I., Lever, V., Porta, G., Riva, M., et al. 2013 *Global sensitivity analysis through polynomial chaos expansion of a basin-scale geochemical compaction model.* Computational Geosciences, 17(1), 25–42.

Modeling Methane and Non-Hydrocarbon Gases Migration in Sedimentary Basins

Alfredo Battistelli
Saipem SpA, AMBEN Dept.
Via Toniolo 1, 61032 Fano (PU) - Italy
alfredo.battistelli@saipem.com

Alberto Consonni
Eni SpA - Upstream and Technical Services
Via F. Maritano 26, 20097 San Donato Milanese (MI) - Italy
alberto.consonni@eni.com

Matilde Dalla Rosa
Eni SpA - Upstream and Technical Services
via Emilia 1, 20097 San Donato Milanese (MI) - Italy
matilde.dalla.rosa@eni.com

Claudio Geloni
Eni SpA - Upstream and Technical Services
Via F. Maritano 26, 20097 San Donato Milanese (MI) - Italy
claudio.geloni@eni.com

Modeling of sedimentary basins evolution is conventionally performed to support the exploration activities of the Oil & Gas industry, aimed at the evaluation of potential hydrocarbon reserves. In particular, it allows to outline the possible hydrocarbons location by simulating fluid flow and migration of related components, such as inorganic gases and brine, in conjunction with the evolution of the basin in terms of sediment deposition and compaction. The migration of hydrocarbons and gases through sedimentary units towards structural traps is simulated either with simplified approaches involving ray-tracing and percolation theory, or with the multiphase Darcy's law able to better capture all relevant processes [4]. We present the first results of an effort to improve the capability of TOUGH2-TMGAS reservoir simulator ([1], [2]) to better describe the physics underlying migration and geochemical reactions of hydrocarbons and inorganic gases (CO_2, H_2S) at basin scale and for geological times.
TMGAS [1] is an EOS module of TOUGH2 reservoir simulator developed to model the thermodynamics and evaluate phase transport properties of hydrocarbons and inorganic gas mixtures in equilibrium with NaCl brines up to halite saturation and at temperature (T) and pressure (P) up to 250 °C and 100 MPa, depending on the gas solubility data to calibrate the EOS. TMGAS has been employed to simulate the migration of CH_4, CO_2 and H_2S generated by natural processes in a portion of a wide sedimentary formation, extending from depths of 2000 to 6800 m, with the aim to evaluate code capabilities and anticipate the needs for code improvements to increase the T limit to 300 °C and enhance the simulation speed. Simulations were performed using stationary spatial grids (no compaction and burial) and by neglecting geochemical reactions which can be simulated

using TOUGHREACT-TMGAS. The simulator was able to model the migration of CH_4, CO_2 and H_2S, alone or as gas mixtures, in fresh and saline aquifers for T and P up to 240 °C and 650 bar and for times up to 5 Myrs. 3D Voronoi unstructured grids, built to conforms to the Integral Finite Difference Method (IFDM) used by TOUGH2, were employed [3] to properly follow the geometry of sedimentary formation.
Simulations highlighted the effects of thermodynamic and transport properties of gases on their distribution among the aqueous (AQ) and non-aqueous (NA) phase and on their migration patterns. Generation of CO_2 and H_2S produce smaller NA plumes due to the high density of NA phase (620-720 kg/m^3) and their high solubility in the AQ phase. On the other hand, CH_4 migrates faster, producing wider NA plumes due to its lower NA phase density (130-170 kg/m^3) and low solubility. Gas dissolution produces an increase of CO_2–saturated brine density and a reduction of H_2S– and CH_4–saturated brine density driving convection flows affecting gas distribution at basin scale.
The control of numerical performances of TMGAS suggested that future code developments should be implemented to *i)* improve the modeling of gas-brine equilibria by calibrating the EOS with more recent mutual solubility data at higher T and P; *ii)* improve the iterative phase equilibria algorithms originally optimized for lower T, thus for lower water contents in the NA phase; *iii)* eliminate the convergence problems, characteristic of TOUGH2 simulator, related to the proper weighting of the gravity contribution to the P gradient in the multiphase version of Darcy's law. Tiny time steps are occasionally required by convergence issues at few grid elements located at the front of advancing NA plume, when its migration is governed by density-driven flow; *iv)* reduce grid effects on the proper modeling of T, P and concentration gradients by using smaller grid spacing and implementing local grid refinement, where necessary.
Local grid refinement is quite easy with the IFDM used by TOUGH2 for spatial discretization of mass and energy balance equations, providing that a suitable grid generator is available [3]. However, both local grid refinement and smaller grid spacing might increase considerably the number of grid elements and then the number of balance equations to be solved. At this respect, Eni SpA developed a parallel version of TOUGH2–TMGAS which will be the basis for future simulation studies of hydrocarbons and inorganic gas mixtures migration within sedimentary basins for geological times.

References

[1] Battistelli A., Marcolini M. 2009 *TMGAS: a new TOUGH2 EOS module for the numerical simulation of gas mixtures injection in geological structures.* Intl. J. Greenhouse Gas Control 3, 481–493.

[2] Battistelli A., Berry P., Bonduà S., Bortolotti V., Consonni A., Cormio C., Geloni C., Vasini E.M. 2015 *Thermodynamics related processes during the migration of acid gases and methane in deep sedimentary formations.* TOUGH Symposium 2015, Sept. 28–30, 2015, Berkeley, CA, USA.

[3] Bonduà S., Battistelli A., Berry P., Bortolotti V., Consonni A., Cormio C., Geloni C., Vasini E.M. 2015 *Voronoi 3D pre- and post-processing tools for the modeling of deep sedimentary formations with the TOUGH2 family of codes.* TOUGH Symposium 2015, Sept. 28–30, 2015, Berkeley, CA, USA.

[4] Oldenburg C.M., Mukhopadhyay S., Cihan A. 2015 *On the use of Darcy's law and invasion-percolation approaches for modeling large-scale geologic carbon sequestration.* Greenhouse Gases Sci. and Tech. 5, 1–15.

Large-scale and Data-driven PDE problems: Uncertainty Quantification & Reduced Order Modeling - Part I

PROPOSERS

Andrea Manzoni
Ecole Polytechnique Fédérale de Lausanne (EPFL)
av. Piccard, Station 8, CH-1015 - Lausanne, Switzerland
andrea.manzoni@epfl.ch

Lorenzo Tamellini
Istituto di Matematica Applicata e Tecnologie Informatiche (IMATI) - CNR
Via Ferrata 1, 27100 - Pavia, Italy
tamellini@imati.cnr.it

SPEAKERS

Andrea Manzoni
MATHICSE-CMCS, EPFL
federico.negri@epfl.ch

Maria Vittoria Salvetti
Dip. Ing. Civile e Industriale, Università di Pisa
mv.salvetti@ing.unipi.it

Federico Negri
MATHICSE-CMCS, EPFL
federico.negri@epfl.ch

Eleonora Musharbash
MATHICSE-CSQI, EPFL
eleonora.musharbash@epfl.ch

Christopher Spannring
Dept. Math., TU Darmstadt
spannring@mathematik.tu-darmstadt.de

Laura M. Sangalli
Dip. Matematica, Politecnico di Milano
laura.sangalli@polimi.it

A growing number of applications in engineering requires to merge mathematical models built on partial differential equations and complex data (possibly high-dimensional and/or affected by uncertainty) in order to perform tasks such as driving a system to a desired target, ensuring minimal operational risk, identifying its unknown features or exploring efficiently different scenarios. Data assimilation, uncertainty quantification, PDE-constrained optimization and inverse problems are therefore becoming more and more the mainstays of modern computational science. However, while recent advances

in reduced order modeling and uncertainty quantification techniques increasingly allow to successfully tackle large-scale problems using computationally tenable algorithms, several outstanding theoretical and algorithmical challenges remain. The purpose of this minisymposium is to bring together researchers who are active in the above-mentioned fields, to present novel and promising methods, and to discuss future trends for research.

Reduced basis methods for parameter identification in PDE problems: reliability and computational efficiency

Andrea Manzoni
CMCS-MATHICSE-SB
Ecole Polytechnique Fédérale de Lausanne,
Station 8, CH-1015 Lausanne, Switzerland
andrea.manzoni@epfl.ch

Alfio Quarteroni
CMCS-MATHICSE-SB
Ecole Polytechnique Fédérale de Lausanne,
Station 8, CH-1015 Lausanne, Switzerland
alfio.quarteroni@epfl.ch

Stefano Pagani
MOX, Dipartimento di Matematica
Politecnico di Milano
P.za Leonardo da Vinci 32, I-20133 Milano, Italy
stefano.pagani@polimi.it

Reduced basis (RB) methods represent a very efficient approach for the numerical approximation of problems involving the repeated solution of differential equations arising from engineering and applied sciences [5]. Noteworthy examples include partial differential equations (PDEs) depending on several parameters, PDE-constrained optimization, optimal control and inverse problems and, more recently, UQ problems. When dealing with these cases several challenges have to be faced to ensure the reliability and the computational efficiency of the RB method.
After an overview on the current state of the art of RB methods for parametrized PDEs, we show how to take advantage of a RB approximation e.g. when dealing with parameter identification for PDE models, where a Bayesian framework can be exploited for the sake of uncertainty quantification. Indeed, sampling techniques such as Monte Carlo Markov Chain (MCMC) or Kalman Filters (in the case of dynamical systems) are computationally demanding, since they usually require a huge number of queries to the forward PDE model [2, 4].
In this respect, efficiency is often ensured by performing a further reduction level, aiming at the approximation of complex nonaffine or nonlinear parametrized operators possibly appearing in the forward problem [3, 1]. On the other hand, reliability is met by a suitable model for those reduction errors – unavoidable when replacing the high-fidelity model with the RB approximation – whose propagation must be controlled for the sake of bias reduction in the resulting parameter estimates. Numerical results will be shown in order to assess the efficacy of the proposed methods.

References

[1] Manzoni, A. and Negri, F. 2016 *Automatic reduction of PDEs defined on domains with variable shape*. Submitted, Mathicse Report N. 19-2016.

[2] Manzoni, A. and Pagani, S. and Lassila, T. 2016 *Accurate solution of Bayesian inverse uncertainty quantification problems combining reduced basis methods and reduction error models*. SIAM/ASA J. Uncertainty Quantification 4, 380–412.

[3] Negri, F. and Manzoni, A. and Amsallem, D. 2015 *Efficient model reduction of parametrized systems by matrix discrete empirical interpolation*. J. Comput. Phys. 303, 31–454.

[4] Pagani, S. and Manzoni, A. and Quarteroni, A. 2016 *A reduced basis ensemble Kalman filter for state/parameter identification in large-scale nonlinear dynamical systems*. Submitted, Mathicse Report N. 18-2016.

[5] Quarteroni, A. and Manzoni, A. and Negri, F. 2016 *Reduced Basis Methods for Partial Differential Equations. An Introduction.* Springer, Unitext Series, vol. 92.

Stochastic sensitivity analysis in numerical simulation of the flow in ascending aorta aneurysms

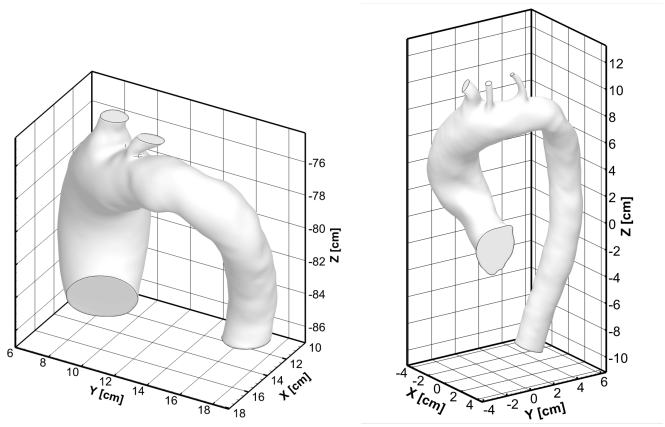
Maria Vittoria Salvetti
Dipartimento di Ingegneria Civile e Industriale, Università di Pisa
Via G. Caruso 8, 56122 Pisa, Italia
mv.salvetti@ing.unipi.it

Alessandro Boccadifuoco
Scuola Superiore Sant'Anna
Piazza Martiri della Libertà 33, 56127 Pisa, Italia
alessandro.boccadifuoco@sssup.it

Alessandro Mariotti
Dipartimento di Ingegneria Civile e Industriale, Università di Pisa
Via G. Caruso 8, 56122 Pisa, Italia
alessandro.mariotti@for.unipi.it

Simona Celi
Fondazione CNR - Regione Toscana G. Monasterio
Via Aurelia Sud, 54100 Massa, Italia
s.celi@ftgm.it

An Ascending Thoracic Aortic Aneurysm (ATAA) is a typical cardiovascular disease that consists in a permanent dilatation of the ascending thoracic aorta and can lead to major complications, like aortic dissection and rupture. Aortic dissection and aortic rupture carry a mortality rate of about 20% and 90%, respectively, whereas surgical intervention has a mortality risk of approximately 5%. Evaluating the risk of ATAA complications is thus of fundamental importance to decide the best possible clinical strategy. The current clinical practice consists in recommending surgery if the maximum aneurysm diameter exceeds 5.5 cm. However, this index alone is not able to describe the biomechanical state of the arterial wall and does not represent a reliable predictor of complications, especially in case of small and medium-sized aneurysms.
Since rupture and dissection can be considered as the effects of preponderant stresses on the structurally compromised wall, the aneurysmatic pathology has been investigated from a biomechanical point of view by modeling the structural behavior of the wall and imposing the value of the pressure inside the aorta. This approach has led to the definition of new indices, e.g. the peak wall stress, which have been shown to outperform the maximum diameter in predicting rupture.
However, these structural studies neglect the impact of the hemodynamics, which is actually believed to play a key role in the origin and evolution of the aneurysms. The literature has pointed out that abnormal flow patterns and, in particular, abnormal wall shear stress have an important effect on the endothelial cells of the artery, possibly altering their morphology, orientation and permeability. In this context, in recent years the simulation of the blood flow by means of Computational Fluid Dynamics (CFD) has



(a) Geometry A (b) Geometry B

Figure 1: Sketch of the considered geometries.

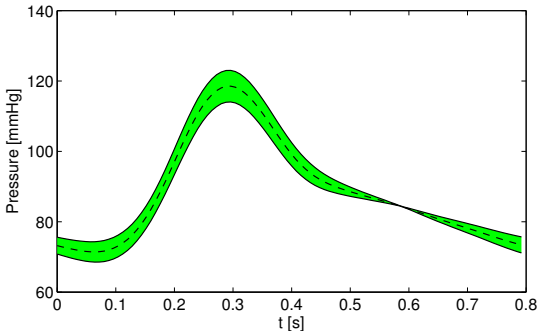
become more and more common, since these techniques allow to quantify a large number of variables that cannot be directly obtained through *in-vivo* measurements. In addition, the combined use of CFD and medical imaging seems to be very promising, as it provides real anatomic data and velocities and thus permits to investigate the hemodynamics on a patient-specific basis.

Nonetheless, reliable patient-specific models are usually difficult to be obtained since CFD requires modeling assumptions that affect the accuracy of the simulations. These assumptions may be seen as sources of uncertainty and a stochastic analysis can be performed in order to evaluate their effect on the quantities of interest. Our work focuses on uncertainties in boundary conditions in patient-specific ATAA geometries, for both rigid and deformable-wall cases. At the inlet we imposed either an idealized flow rate waveform or patient-specific data coming from *in-vivo* measurements. At the outlets the choice is more challenging, since outflow boundary conditions should model what happens outside the computational domain. A widespread practice is to use lumped parameter models that characterize the effect of downstream organs and vessels by means of resistance, capacitance and inductance, according to the electric analogy between voltage and blood pressure and between current and flow rate. We chose the three-element Windkessel model, thus modeling the small vessels with a distal resistance and the large vessels by means of a proximal resistance and a capacitance. The present Uncertainty Quantification (UQ) analysis focuses on uncertainties in the value of these three parameters as well.

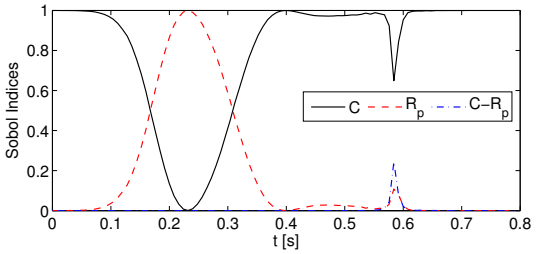
We considered two patient-specific geometries of thoracic aortas, characterized by different severity of ATAA: the first aneurysm has a maximum diameter of 5.1 cm, the second one a maximum diameter of 3.8 cm (Figure 1).

The hemodynamic simulations were performed with *SimVascular*, an open-source package specific for cardiovascular applications. We used unstructured tetrahedral grids for their adaptability to complex computational domains, and grid independence was checked on the values of the following quantities: maximum value of Wall Shear Stress (WSS) and velocity at various time instants, and maximum value of Time-Averaged Wall Shear Stress (TAWSS). Both rigid and deformable-wall simulations were performed. When considering the arterial wall compliance, for the sake of simplicity the aorta was assumed to be elastic, homogeneous and isotropic, with a uniform wall thickness.

As for the stochastic approach, we used the generalized Polynomial Chaos method with uniform probability density distributions and, thus, Legendre orthogonal polynomials.



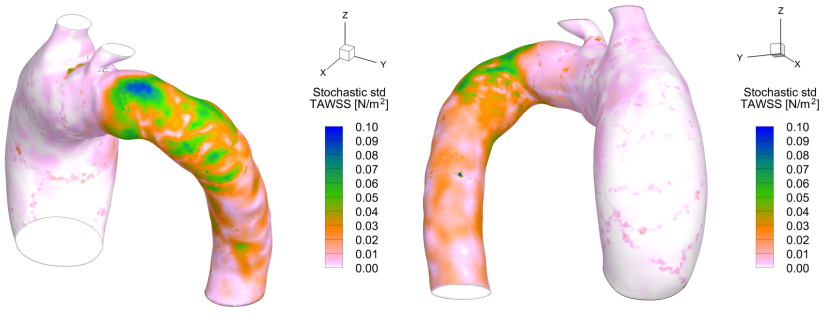
(a)



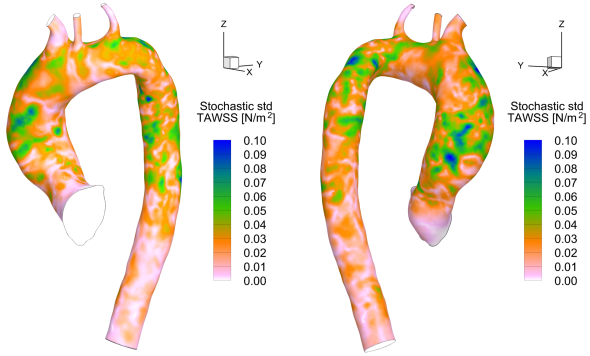
(b)

Figure 2: Effect of the uncertainties in the capacitance C and proximal resistance R_p on the pressure waveform in correspondence of the descending aorta outlet section (geometry A with rigid walls). The results are expressed in terms of stochastic mean ± stochastic standard deviation (a) and partial sensitivities to the two parameters (b).

Since a preliminary analysis showed that the proximal resistance and the capacitance are the main parameters affecting the pressure waveform in the 0D Windkessel model, these two quantities were selected as uncertain parameters for the UQ analysis, whereas a fixed physiological value of the distal resistance was maintained.
We analyzed the impact of the considered uncertainties on the pressure waveform at the descending aortic outlet section, as well as on the following hemodynamic descriptors: WSS, TAWSS, Oscillatory Shear Index (OSI). Our results show that the stochastic mean values of the quantities above are in general very similar to the values obtained in the deterministic simulations carried out with guessed values of the outflow parameters. For the case with two sources of uncertainty, Figure 2 shows the pressure waveform in terms of the stochastic mean value ± the stochastic standard deviation, together with the partial sensitivities to the two uncertain parameters along a cardiac cycle: for most part of the cycle C is the main responsible of the variability of the results, R_p becoming predominant in a small portion near peak systole.
The variability of the hemodynamic descriptors was found to depend on the geometry considered, being much larger in the small aneurysm (Figure 3). In addition, taking into account the wall compliance reduces the impact of the uncertainties in the outflow parameters (Figure 4). A similar stochastic sensitivity analysis to uncertainties in the inlet flow rate waveform is in progress and the results will be shown in the final presentation.

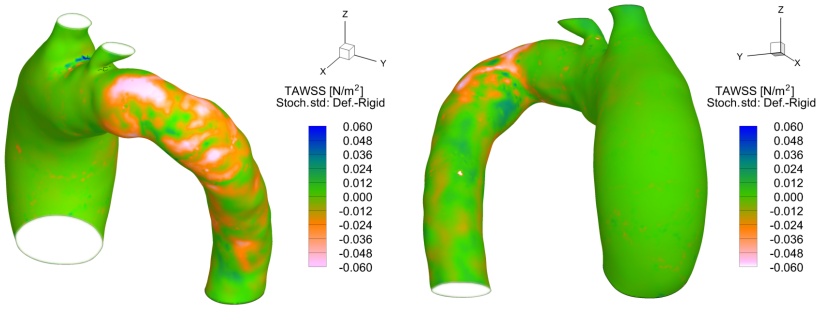


(a) Front view (b) Back view



(c) Front view (d) Back view

Figure 3: Stochastic standard deviation of TAWSS for the geometry A (a-b) and geometry B (c-d) (rigid walls). Effect of uncertainties in the value of the capacitance C.



(a) Front view (b) Back view

Figure 4: Effect on the TAWSS distribution of uncertainties in the value of the capacitance C (geometry A with deformable walls): difference between the stochastic standard deviations in deformable and rigid cases.

Efficient techniques for the model order reduction of parametrized problems in computational fluid and solid mechanics

Federico Negri
École polytechnique fédérale de Lausanne
Av. Piccard, Station 8, 1015 Lausanne, Switzerland
federico.negri@epfl.ch

Since the high-fidelity approximation of many complex models easily leads to solve large-scale problems, the need to perform multiple simulations to explore different scenarios, as well as to achieve rapid responses, often requires unaffordable computational resources. Alleviating this extreme computational effort represents the main motivation for developing ROMs, i.e. low-dimensional approximations of the underlying high-fidelity problem.
Among a wide range of model order reduction approaches, here we focus on the so-called projection-based methods [1]. In this context, the goal is to generate low cost and fast, but still sufficiently accurate ROMs which characterize the system response for the whole range of input parameters we are interested in. In particular, several challenges have to be faced to ensure reliability and computational efficiency. Concerning this latter, we propose and compare different strategies to combine the Discrete Empirical Interpolation Method (DEIM) and its matrix variant with a state approximation resulting either from a proper orthogonal decomposition or a greedy approach [2, 3]. Specifically, we exploit these techniques to develop fast and efficient ROMs for nonaffinely parametrized and nonlinear problems arising in computational solid and fluid dynamics, as well as in fluid-structure interaction. In all these cases, high performance computing plays a central role in both the design and implementation of the algorithms used to train (offline) and rapidly evaluate (online) the ROM [4].
The efficacy of the proposed methods is demonstrated on a variety of computationally-intensive applications, such as the prediction of wall stresses in abdominal aortic aneurysms and the simulation of coupled blood flow and mass transport in human arteries.

References

[1] A. Quarteroni, A. Manzoni, and F. Negri. *Reduced Basis Methods for Partial Differential Equations. An Introduction*. Springer International Publishing, Switzerland, 2016.

[2] F. Negri. *Efficient Reduction Techniques for the Simulation and Optimization of Parametrized Systems: Analysis and Applications*. PhD thesis, EPFL, Lausanne, 2015.

[3] F. Negri, A. Manzoni, and D. Amsallem. *Efficient model reduction of parametrized systems by matrix discrete empirical interpolation*. J. Comp. Phys., 2015.

[4] D. Forti, F. Negri. *A high performance computing framework for the model order reduction of nonlinear structural problems in biomechanics*. In preparation, 2016.

Dynamical low rank approximation of time dependent PDEs with random parameters

Eleonora Musharbash
École Polytechnique Fédérale de Lausanne
Station 8, CH-1015 Lausanne, Switzerland
eleonora.musharbash@epfl.ch

Fabio Nobile
École Polytechnique Fédérale de Lausanne
Station 8, CH-1015 Lausanne, Switzerland
fabio.nobile@epfl.ch

Many physical and engineering problems can be properly described by mathematical models, typically of differential type. However, in many situations, the input parameters may be affected by uncertainty due e.g. to measurement errors, limited data availability or intrinsic variability of the phenomenon itself. A convenient way to characterize uncertainty consists in describing the uncertain parameters as random variables or space and/or time varying random fields.
In this talk, we consider a general (linear or non linear) time dependent partial differential equation (PDE) with random parameters in which the randomness can appear in the operator as a random parameter or forcing term as well as in the initial datum or boundary condition. Our goal is to approximate the solution in a low dimensional manifold. We consider the Dynamical Low Rank approximation method, in the same spirits of what proposed in [1] for the approximation of a deterministic evolution matrix equation, and [3] in the Uncertainty Quantification framework. This approach consists in a reduced basis method according to which the approximate solution is written in a separable form as a linear combination of a small (fixed) number of deterministic basis functions with stochastic coefficients, with the peculiarity that both the basis functions and the coefficients evolve in time. From a variational point of view the approximate solution is sought in the low dimensional manifold of fixed rank S and is obtained by performing a Galerkin projection of the governing equations onto the (time-dependent) tangent space to the manifold along the solution trajectory. After an explicit parametrization of the manifold, one obtains a set of nonlinear differential equations, suitable for numerical integration, for both the coefficients and the basis functions of the approximate solution. In particular we discuss the application of the Dynamical Low Rank technique to the incompressible Navier Stokes equations with random boundary conditions. With this purpose we derive a slightly different formulations, named dual Dynamically Orthogonal (dual DO) formulation, that better deals with divergence free constraints as well as non-homogeneous random boundary conditions. The method proposed is tested on a hemodynamic problem, in which the blood flow is simulated in a realistic carotid artery reconstructed from MRI imaging. We assumed random inflow conditions due to uncertainty in Doppler measurements of the inflow velocity.
We will also discuss possible extensions of the Dynamical Low Rank approach for the approximation of second order wave equations with random parameters.

References

[1] O. Koch, C. Lubich, Dynamically low-rank approximation, SIAM J. Matrix Anal.Appl., Vol.29, No.2(2007), pp.434-454.

[2] E. Musharbash, F. Nobile, T. Zhou, Error analysis of the Dynamical Orthogonal approximation of time dependent random PDEs. SIAM Journal on Scientific Computing 37 (2) A776 (2015),DOI: 10.1137/140967787

[3] T. P. Sapsis and P. F.J. Lermusiaux, Dynamically orthogonal field equations for continuous stochastic dynamical systems, Physica D, 238 (2009) 2347-2360.

Reduced Basis Method for Parabolic Problems with Random Data

Christopher Spannring
TU Darmstadt, Graduate School CE
Dolivostraße 15, 64293 Darmstadt, Germany
spannring@gsc.tu-darmstadt.de

Sebastian Ullmann
TU Darmstadt, Graduate School CE
Dolivostraße 15, 64293 Darmstadt, Germany
ullmann@gsc.tu-darmstadt.de

Jens Lang
TU Darmstadt, Graduate School CE
Dolivostraße 15, 64293 Darmstadt, Germany
lang@mathematik.tu-darmstadt.de

In the talk we consider the reduced basis method applied to a time dependent PDE problem with uncertain input. Uncertainties in PDE models may arise from lack of knowledge regarding geometry, boundary conditions, source terms or model coefficients. In this context, one is often interested in statistics of functionals of the solution, rather than in the solution itself.
We treat the uncertainty by the Monte Carlo (MC) method [5] where the PDE needs to be solved for N_{MC} randomly chosen parameter samples. MC is attractive since it is easy to implement and its convergence rate is independent of the stochastic parameter dimension. However, a large number of samples N_{MC} is required in order to achieve reasonable accuracy because of the low convergence rate of $\mathcal{O}(N_{MC}^{-1/2})$. For each sample a PDE problem needs to be solved, which is computationally expensive with standard numerical discretization methods.
The reduced basis method approximates the solution manifold (over the parameters) on a low-dimensional subspace, which is constructed by the greedy procedure [1]. The method yields a rigorous a posteriori error estimator for the error between the finite element and the reduced solution. The focus of this talk is the consideration of linear output functionals and their error estimation. A primal-dual approach is considered, which uses the solution of an adjoint problem, see [6].
As a numerical example, we study a time dependent heat problem as described in [3], where a heat flow on a heat shield is analyzed. The domain includes three squared cooling channels, see Figure 1.

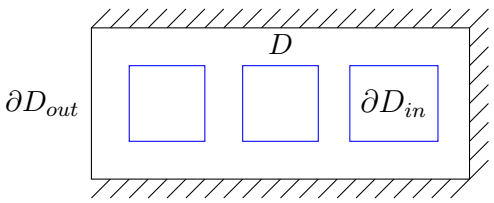


Figure 1: Heat flow in domain D with cooling channels (blue)

The variational formulation of the considered instationary heat problem is given as follows: find $u \in H^1(D)$ such that

$$\int_D \partial_t uv + \int_D \nabla u \cdot \nabla v + \xi_1 \int_{\partial D_{out}} uv + \xi_2 \int_{\partial D_{in}} uv = \xi_1 \int_{\partial D_{out}} vg(t), \quad \forall v \in H^1(D),$$

where u denotes the unknown temperature field. Discretization in space is done by linear finite elements and the implicit Euler method is used for time integration. In [3] a pure greedy procedure is implemented in order to choose optimal parameter samples. The solutions for these samples span the reduced basis space. A low-dimensional reduced system is derived by Galerkin projection. The output of interest is the average temperature in the domain, $l(v) = |\Omega|^{-1} \int_\Omega v$. Since the functional is chosen differently from the right hand side, this is the so called non-compliant case, see [6]. We present the following extensions to the example of [3]:

- We replace the pure greedy procedure by the POD-greedy method [4] for the time and the parameter selection, yielding a smaller RB space dimension.
- The heat transfer coefficient ξ_2 is modeled by a random variable and hence the solution as well as the output functional is a random quantity.
- Statistical quantities are estimated with the help of the reduced system and the MC method.
- We implement a weighted reduced basis method [2] in order to minimize the error in the expectation.

References

[1] A. Buffa, Y. Maday, A. T. Patera., C. Prud'homme and G. Turinici. *A priori convergence of the greedy algorithm for the parametrized reduced basis method*. ESAIM Math. Model. Numer. Anal., 46(3):595–603, 2012.

[2] P. Chen, A. Quarteroni and G. Rozza. *A weighted reduced basis method for elliptic partial differential equations with random input data*. SIAM J. Numer. Anal., 51(6):3163–3185, 2013.

[3] M. A. Grepl and A. T. Patera. *A posteriori error bounds for reduced-basis approximations of parametrized parabolic partial differential equations*. M2AN Math. Model. Numer. Anal., 39(1):157–181, 2005.

[4] B. Haasdonk and M. Ohlberger. *Reduced basis method for finite volume approximations of parametrized linear evolution equations*. M2AN Math. Model. Numer. Anal., 42(7):277–302, 2008.

[5] M. Papadrakakis and V. Papadopoulos. *Robust and efficient methods for stochastic finite element analysis using Monte Carlo simulation*. CMAME, 134(3–4):325–340, 1996.

[6] C. Prud'homme, D.V. Rovas, K. Veroy, L. Machiels, Y. Maday, A. T. Patera and G. Turinici. *Reliable real-time solution of parametrized partial differential equations: reduced-basis output bound methods*. ASME. J. Fluids Eng., 124(1):70–80, 2001.

PDE regularized principal component analysis on bidimensional manifolds, with applications to neuroimaging data

Laura M. Sangalli
MOX- Dipartimento di Matematica, Politecnico di Milano
Piazza L. da Vinci 32, 20133 Milano, Italy
laura.sangalli@polimi.it

Eardi Lila
Cambridge Centre for Analysis, University of Cambridge
The Old Schools, Trinity Lane, Cambridge CB2 1TN UK
el425@cam.ac.uk

John A.D. Aston
Statistical Laboratory, University of Cambridge
The Old Schools, Trinity Lane, Cambridge CB2 1TN UK
j.aston@statslab.cam.ac.uk

Motivated by the analysis of high-dimensional neuroimaging signals over the cerebral cortex, we introduce a principal component analysis technique that can be used for exploring the variability and for performing dimensional reduction of signals observed over two-dimensional manifolds. The proposed method is based on a PDE regularization approach, involving the Laplace-Beltrami operator associated to the manifold domain. The model introduced can be applied to data observed over any two-dimensional manifold topology, and can naturally handle missing data and signals evaluated in different grids of points. The proposed method is applied to the analysis of resting state functional magnetic resonance imaging data from the Human Connectome Project.

This method is illustrated in [6] and has been developed within a line of research

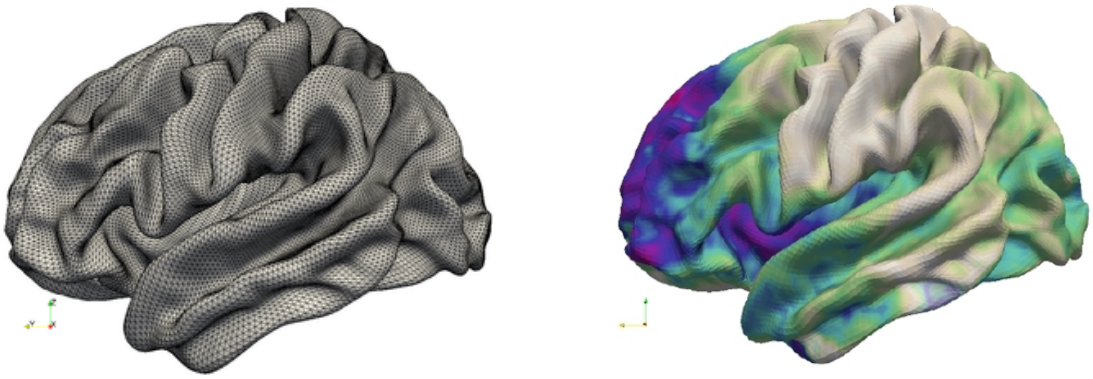


Figure 1: Left: a triangulated surface approximating the left hemisphere of the cerebral cortex, a highly convoluted thin sheet of neural tissue that constitutes the outermost part of the brain. Right: hemodynamical signal associated to neural activity over the cerebral cortex.

concerning spatial regression with differential regularizations [1, 2, 3, 4, 5, 8, 9, 10]. The implementation of the method is based on the R package fdaPDE [7] released via The Comprehensive R Archive Network.

References

[1] Azzimonti, L., Nobile, F., Sangalli, L.M., Secchi, P. 2014 *Mixed Finite Elements for spatial regression with PDE penalization*, SIAM/ASA Journal on Uncertainty Quantification, Vol. 2 (1), pp. 305–335.

[2] Azzimonti, L., Sangalli, L.M., Secchi, P., Domanin, M., Nobile, F. 2015 *Blood flow velocity field estimation via spatial regression with PDE penalization*, Journal of the American Statistical Association, Theory and Methods, Vol. 110 (511), pp. 1057–1071.

[3] Bernardi, M.S., Sangalli, L.M., Mazza, G., Ramsay, J.O. 2016 *A penalized regression model for spatial functional data with application to the analysis of the production of waste in Venice province*, Stochastic Environmental Research and Risk Assessment, DOI: 10.1007/s00477-016-1237-3.

[4] Dassi, F., Ettinger, B., Perotto, S., Sangalli, L.M. 2015 *A mesh simplification strategy for a spatial regression analysis over the cortical surface of the brain*, Applied Numerical Mathematics, Vol. 90 (1), pp. 111–131.

[5] Ettinger, B., Perotto, S., Sangalli, L.M. (2016). *Spatial regression models over two-dimensional manifolds*, Biometrika, Vol. 103 (1), pp. 71–88.

[6] Lila, E., Aston, J.A.D., Sangalli, L.M. 2016. *Smooth Principal Component Analysis over two-dimensional manifolds with an application to Neuroimaging*, ArXiv:1601.03670, http://arxiv.org/abs/1601.03670.

[7] Lila, E., Sangalli, L.M., Ramsay, J.O., Formaggia, L. 2016 *fdaPDE: functional data analysis and Partial Differential Equations; statistical analysis of functional and spatial data, based on regression with partial differential regularizations*, R package version 0.1-4,
http://CRAN.R-project.org/package=fdaPDE.

[8] Sangalli, L.M., Ramsay, J.O., Ramsay, T.O. 2013, *Spatial spline regression models*, Journal of the Royal Statistical Society Ser. B, Statistical Methodology, Vol. 75 (4), pp. 681–703.

[9] Wilhelm, M., Sangalli, L.M. 2016, *Generalized Spatial Regression with Differential Regularization*, Journal of Statistical Computation and Simulation, DOI: 10.1080/00949655.2016.1182532.

[10] Wilhelm, M., Dede', L., Sangalli, L.M., Wilhelm, P. 2016 *IGS: an IsoGeometric approach for Smoothing on surfaces*, Computer Methods in Applied Mechanics and Engineering, Vol. 302, pp. 70–89.

Large-scale and Data-driven PDE problems: Uncertainty Quantification & Reduced Order Modeling - Part II

PROPOSERS

Andrea Manzoni
Ecole Polytechnique Fédérale de Lausanne (EPFL)
av. Piccard, Station 8, CH-1015 - Lausanne, Switzerland
andrea.manzoni@epfl.ch

Lorenzo Tamellini
Istituto di Matematica Applicata e Tecnologie Informatiche (IMATI) - CNR
Via Ferrata 1, 27100 - Pavia, Italy
tamellini@imati.cnr.it

SPEAKERS

Fabio Nobile
MATHICSE-CSQI, EPFL
fabio.nobile@epfl.ch

Stefano Mariani
Politecnico di Milano, Dipartimento di Ingegneria Civile e Ambientale
stefano.mariani@polimi.it

Christophe Prud'homme
Advanced Math. Res. Inst., Univ. Strasbourg
prudhomme@unistra.fr

Lorenzo Tamellini
IMATI-CNR
tamellini@imati.cnr.it

Niccolò Dal Santo
MATHICSE-CMCS, EPFL
niccolo.dalsanto@epfl.ch

Andrea Serani
INSEAN-CNR
andrea.serani@insean.cnr.it

A growing number of applications in engineering requires to merge mathematical models built on partial differential equations and complex data (possibly high-dimensional and/or affected by uncertainty) in order to perform tasks such as driving a system to a desired target, ensuring minimal operational risk, identifying its unknown features or exploring efficiently different scenarios. Data assimilation, uncertainty quantification, PDE-constrained optimization and inverse problems are therefore becoming more and more the mainstays of modern computational science. However, while recent advances

in reduced order modeling and uncertainty quantification techniques increasingly allow to successfully tackle large-scale problems using computationally tenable algorithms, several outstanding theoretical and algorithmical challenges remain. The purpose of this minisymposium is to bring together researchers who are active in the above-mentioned fields, to present novel and promising methods, and to discuss future trends for research.

Advances on multi level Monte Carlo methods for random PDEs

Fabio Nobile
CSQI-MATHICSE, École Polytechnique Fédérale de Lausanne
CH-1015, Lausanne, Switzerland
fabio.nobile@epfl.ch

Michele Pisaroni
CSQI-MATHICSE & IAG-IGM, École Polytechnique Fédérale de Lausanne
CH-1015, Lausanne, Switzerland
michele.pisaroni@epfl.ch

Pénélope Leyland
IAG-IGM, École Polytechnique Fédérale de Lausanne
CH-1015, Lausanne, Switzerland
penelope.leyland@epfl.ch

Francesco Tesei
CSQI-MATHICSE, École Polytechnique Fédérale de Lausanne
CH-1015, Lausanne, Switzerland
francesco.tesei86@gmail.com

Multi Level Monte Carlo (MLMC) is an emerging technology to effectively compute statistics of the solution of differential problems that include random terms. It can considerably improve the performance of standard Monte Carlo simulations by exploiting a hierarchy of spatial or temporal discretizations of the underlying differential problem and has been successfully applied in several contests.
We focus here on models based on Partial Differential Equations with partially unknown input parameters, modeled as random variables. The setup of a MLMC algorithm, however, includes the choice of a set of parameters that should be properly tuned to achieve optimal performances.
We present a Continuation MLMC algorithm that solves the given approximation problem for a sequence of decreasing tolerances and adaptively calibrates these parameters for the problem at hand. The continuation algorithm is then applied to aerodynamic flows in uncertain operating conditions and geometries.
We will also present application of MLMC to a subsurface flow problem in a random, possibly rough, heterogeneous porous medium. In this case the performance of the MLMC can further be improved by introducing a control variate obtained by a smoothed version of the subsurface problem.

References

[1] M. Pisaroni, F. Nobile and P. Leyland, *A Continuation Multi Level Monte Carlo (C-MLMC) for Uncertainty Quantification in Compressible Aerodynamics.* In prepa-

ration.

[2] F. Nobile and F. Tesei, "A multi level Monte Carlo method with control variate for elliptic PDEs with log-normal coefficients," *Stoch. PDEs: Anal. & Comp.*, vol. 3, no. 3, pp. 398–444, 2015.

Adaptive POD-based reduced order modeling and identification of nonlinear structural systems

Stefano Mariani
Politecnico di Milano, Dipartimento di Ingegneria Civile e Ambientale
Piazza Leonardo da Vinci 32, 20133 - Milano (Italy)
stefano.mariani@polimi.it

Giovanni Capellari
Politecnico di Milano, Dipartimento di Ingegneria Civile e Ambientale
Piazza Leonardo da Vinci 32, 20133 - Milano (Italy)

Alberto Corigliano
Politecnico di Milano, Dipartimento di Ingegneria Civile e Ambientale
Piazza Leonardo da Vinci 32, 20133 - Milano (Italy)

Saeed Eftekhar Azam
Politecnico di Milano, Dipartimento di Ingegneria Civile e Ambientale
Piazza Leonardo da Vinci 32, 20133 - Milano (Italy)

The health monitoring of structures and infrastructures exposed to aging and/or extreme loading conditions is increasingly recognized as a timely issue, not only in civil engineering. To move towards real-time structural health monitoring (SHM) procedures, the adoption of reduced-order models (ROMs) obtained through proper orthogonal decomposition (POD) was proposed in [4]. In the case of a changing structural health, the ROM would need to be continuously re-trained so as to prevent the results to be affected by biases. In [2] a procedure was offered to avoid such time consuming re-training stages; in this work, we further discuss the proposed framework. The chance to attain even larger speedups through a coupling of such reduced-order modeling procedure and adaptive domain decomposition strategies, see e.g. [3], will be also commented during the Conference.
Let us consider a space-discretized (e.g. through finite elements) structural system; its undamped equations of motion read:

$$\mathbf{M}\ddot{\mathbf{u}} + \mathbf{K}\mathbf{u} = \mathbf{f} \tag{1}$$

where: $\mathbf{M}$ and $\mathbf{K}$ are the mass and stiffness matrices of the system; a superposed dot denotes time differentiation; $\ddot{\mathbf{u}}$ and $\mathbf{u}$ are the acceleration and displacement vectors; $\mathbf{f}$ is the external load vector. In case of nonlinear, dissipative events affecting the structural properties, $\mathbf{K}$ may become a function of the current displacements in $\mathbf{u}$.
By partitioning the time interval of interest according to $[t_0 \quad t_{end}] = \cup_{k=1}^{N_t}[t_{k-1} \quad t_k]$ and adopting a standard Newmark integration procedure, the state-space form of Eq. (1) can be written, within a stochastic frame, as:

$$\mathbf{x}_k = \mathbf{A}_k(\boldsymbol{\vartheta}, \boldsymbol{\varphi})\mathbf{x}_{k-1} + \mathbf{v}_k^x \tag{2}$$
$$\mathbf{y}_k = \mathbf{C}_k(\boldsymbol{\varphi})\mathbf{x}_k + \mathbf{v}_k^y \tag{3}$$

where: $\mathbf{x}_k$ represents the whole state of the system at instant t_k, collecting at least the current $\ddot{\boldsymbol{u}}_k$ and $\boldsymbol{u}_k$ vectors; $\mathbf{y}_k$ is the observation vector at t_k; $\mathbf{v}_k^x$ and $\mathbf{v}_k^y$ respectively represent the uncertainties in the process and observation equations; $\boldsymbol{\vartheta}$ and $\boldsymbol{\varphi}$ are two sets of model parameters to be estimated; $\mathbf{A}_k(\boldsymbol{\vartheta}, \boldsymbol{\varphi})$ maps the state of the system within the time step $[t_{k-1} \quad t_k]$; $\mathbf{C}_k(\boldsymbol{\varphi})$ links the observation vector to the state of the system. In Eqs. (2) and (3), for ease of notation the effects of the known exogenous input (if any) have been dropped. System parameters are arranged into the two sets $\boldsymbol{\vartheta}$ and $\boldsymbol{\varphi}$, depending on their physical interpretation: parameters in $\boldsymbol{\vartheta}$ are the uncertainties in the model related to its behavior; parameters in $\boldsymbol{\varphi}$ come instead from a ROM of the system. In the approach here discussed, the ROM can be updated by the procedure whenever necessary (also due to accuracy reasons), taking advantage of the observations in $\mathbf{y}_k$, without the need of a re-training.

As proposed in [4, 2], instead of handling altogether the system vectors $\mathbf{x}_k$, $\boldsymbol{\vartheta}_k$ and $\boldsymbol{\varphi}_k$ (where, as far as vectors $\boldsymbol{\vartheta}$ and $\boldsymbol{\varphi}$ are concerned, the newly-introduced index k identifies the current values provided by the procedure), the problem of dual system identification and ROM update is split into two different stages. First, state and model parameters are dealt with simultaneously, and the relevant state-space model becomes:

$$\begin{Bmatrix} \mathbf{x}_k \\ \boldsymbol{\vartheta}_k \end{Bmatrix} = \begin{bmatrix} \mathbf{A}_k(\boldsymbol{\vartheta}_{k-1}, \hat{\boldsymbol{\varphi}}_{k-1}) & \mathbf{0} \\ \mathbf{0} & \mathbf{I} \end{bmatrix} \begin{Bmatrix} \mathbf{x}_{k-1} \\ \boldsymbol{\vartheta}_{k-1} \end{Bmatrix} + \begin{Bmatrix} \mathbf{v}_k^x \\ \mathbf{v}_k^\vartheta \end{Bmatrix} \tag{4}$$

$$\mathbf{y}_k = \begin{bmatrix} \mathbf{C}_k(\hat{\boldsymbol{\varphi}}_{k-1}) & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \mathbf{x}_k \\ \boldsymbol{\vartheta}_k \end{Bmatrix} + \mathbf{v}_k^y \tag{5}$$

where a hat denotes the estimated values; accordingly, $\hat{\boldsymbol{\varphi}}_{k-1}$ is the vector gathering the estimated features of the ROM at the beginning of the time step. In Eq. (4), since entries of vector $\boldsymbol{\vartheta}_k$ are assumed to be material-dependent, their evolution has been modeled as a random walk with noise term $\mathbf{v}_k^\vartheta$. Second, by assuming the mapping $\mathbf{C}_k$ to be a linear function of $\boldsymbol{\varphi}_k$, the state-space model for $\boldsymbol{\varphi}_k$ itself is stated as:

$$\boldsymbol{\varphi}_k = \boldsymbol{\varphi}_{k-1} + \mathbf{v}_k^\varphi \tag{6}$$

$$\mathbf{y}_k = \mathbf{C}_k^\varphi(\mathbf{x}_k)\boldsymbol{\varphi}_k + \mathbf{v}_k^y \tag{7}$$

where Eq. (7) is a re-formulation of Eq. (3) to explicitly highlight the primary variable $\boldsymbol{\varphi}_k$, in place of $\mathbf{x}_k$. For linear systems, in compliance with Eqs. (4) and (5) the dual estimation of $\mathbf{x}_k$ and $\boldsymbol{\vartheta}_k$ turns out to be nonlinear (actually bi-linear) due to the dependence of mapping $\mathbf{A}_k$ on the state variables $\boldsymbol{\vartheta}_{k-1}$; Eqs. (6) and (7) provide instead a linear state-space model for $\boldsymbol{\varphi}_k$. Thanks to the splitting introduced here above, the full dual system identification problem is handled by a hybrid particle-Kalman filter [5] in the first stage, and by a Kalman filter in the second stage. For nonlinear systems characterized by a reduction of their strength and/or stiffness properties due to damage evolution, mapping $\mathbf{A}_k$ becomes nonlinear by itself; anyhow, provided that system dynamics and damage evolution are characterized by well-separated time-scales, $\mathbf{A}_k$ can be linearized and so assumed constant within each time step, see [2].

To speedup the analysis and allow SHM in real time or at least to move towards that goal, depending on the complexity of the structural system, POD is exploited to build a reduced-order model of the system according to:

$$\boldsymbol{\mathcal{M}}_k = \boldsymbol{\Phi}_k^{\mathrm{T}} \mathbf{M} \boldsymbol{\Phi}_k \qquad \boldsymbol{\mathcal{K}}_k = \boldsymbol{\Phi}_k^{\mathrm{T}} \mathbf{K} \boldsymbol{\Phi}_k \tag{8}$$

where $\boldsymbol{\mathcal{M}}_k$ and $\boldsymbol{\mathcal{K}}_k$ are the ROM mass and stiffness matrices, obtained through matrix $\boldsymbol{\Phi}_k$ collecting the current estimation of the proper orthogonal modes (POMs) given by the

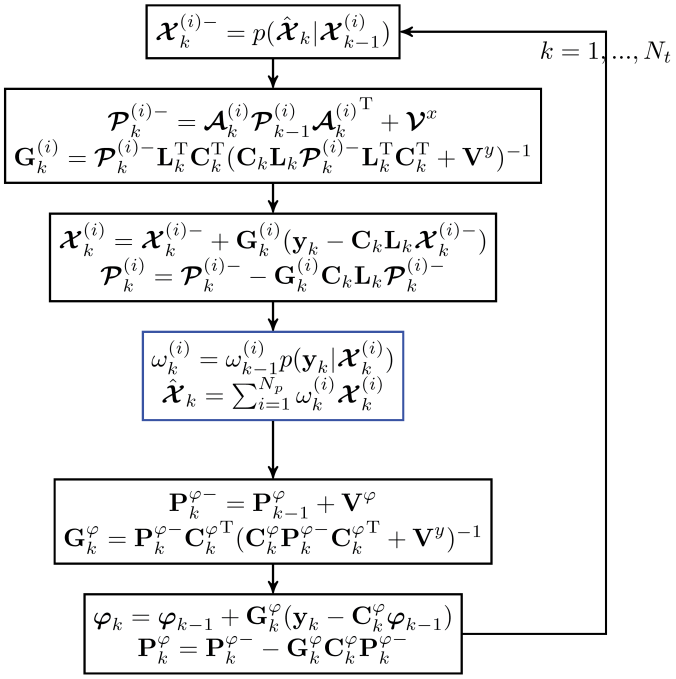


Figure 1: Flow chart of the procedure used for dual estimation and ROM update.

Kalman filter, see [2]. Thanks to Eq. (8), the dual system identification and adaptive ROM problem is pursued within each time step as reported in Figure 1, where: mapping $\boldsymbol{\mathcal{A}}_k^{(i)}$ acts as $\mathbf{A}_k$ in Eq. (4) to evolve the $(i)-$th filter particle; $\boldsymbol{\mathcal{X}}_k^{(i)}$ is the realization of the ROM state provided by the $(i)-$th particle; $\boldsymbol{\mathcal{P}}_k^{(i)}$ is the relevant covariance matrix; $\boldsymbol{\mathcal{V}}^x$ is the noise covariance relevant to the projected state equation; matrix $\mathbf{L}_k = \mathrm{diag}[\boldsymbol{\Phi}_k \quad \boldsymbol{\Phi}_k \quad \boldsymbol{\Phi}_k \quad \mathbf{0}]$ is necessary to link the observations to the ROM state; $\boldsymbol{\varphi}_k$ collects the POMs in vector form; particle weights $\omega_k^{(i)}$ are evolved in time through a multivariate Gaussian distribution $p(\mathbf{y}_k|\boldsymbol{\mathcal{X}}_k^{(i)})$; $\mathbf{G}_k^{(i)}$ and $\mathbf{G}_k^{\varphi}$ are, respectively, the Kalman gains computed in the two stages of the approach to update the estimates $\hat{\boldsymbol{\mathcal{X}}}_k$ and $\boldsymbol{\varphi}_k$.

The proposed approach has been adopted to estimate the damage state of a square thin aluminum plate (characterized by a sidelength/thickness ratio of 40), fully supported along its boundary. For SHM purposes, the structure has been divided into four regions, each one featuring a damage index d_i, $i = 1, ..., 4$, linearly scaling the structural stiffness; such damage indices are collectively gathered in $\boldsymbol{\vartheta}$ and then identified. Observations in $\mathbf{y}_k$ have been assumed the rotations (as a plate kinematics has been adopted for the full-order model, both displacements and rotations are gathered in $\mathbf{u}_k$) measured at the mid-points along the four edges of the plate; these positions were already recognized in [1] as optimal, to reduce the number of sensors to be deployed and maximize the sensitivity of the SHM system. After an initial training stage, state tracking, damage identification and ROM update have been carried out. Since the state is partially observed, the filters perform rather well in tracking system evolution. As for the structural stiffness affected by different damage indices d_i in the four plate regions, exemplary results are reported in Figure 2 at varying order o of the ROM, i.e. at varying number of the retained POMs. It is shown that, while for $o = 1$ and $o = 2$ some biased estimates have been obtained, for $o = 3$ an unbiased estimate of the whole damage state can be promptly obtained. Furthermore, the fast convergence of the local stiffness values E_i proves that the methodology performs

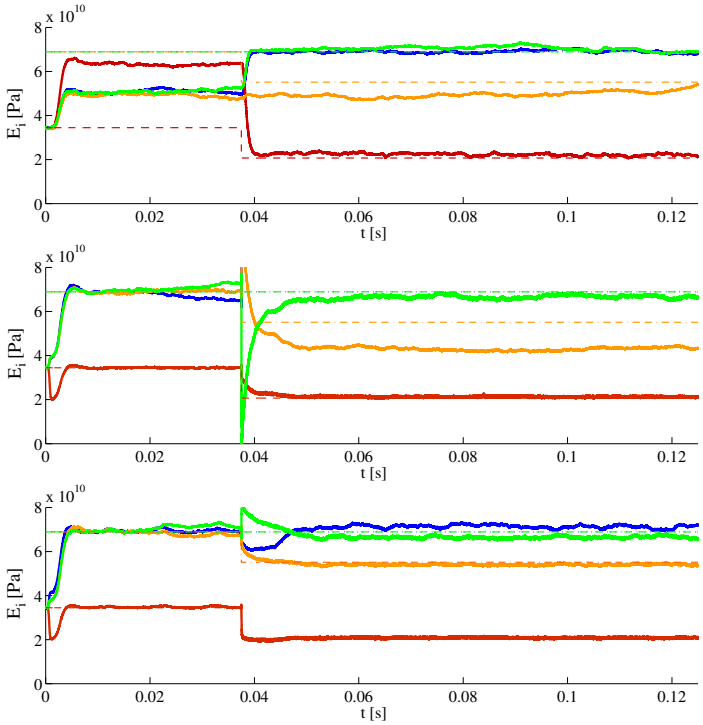


Figure 2: Damaged plate: evolution of the estimated stiffness values E_i in the four plate regions, at varying number of POMs: from top to bottom $o = 1$, $o = 2$ and $o = 3$.

well as for the adaption of the ROM soon after the structural health has changed (in the example at $t = 0.0375$ s); in fact, if ROM update were not carried out, estimations of E_i would easily get biased or even diverge.

Acknowledgement

Partial financial support by Fondazione Cariplo through project *Safer Helmets* is gratefully acknowledged.

References

[1] Bruggi, M. and Mariani, S. 2013 *Optimization of sensor placement to detect damage in flexible plates*. Engineering Optimization 45, 659–676.

[2] Capellari, G., Eftekhar Azam, S. and Mariani, S. 2016 *Damage detection in flexible plates through reduced-order modeling and hybrid particle-Kalman filtering*. Sensors 16, 2.

[3] Corigliano, A., Dossi, M. and Mariani, S. 2015 *Model order reduction and domain decomposition strategies for the solution of the dynamic elasto-plastic structural problem*. Computer Methods in Applied Mechanics and Engineering 290, 127–155.

[4] Eftekhar Azam, S. 2014 *Online Damage Detection in Structural Systems*. Springer.

[5] Eftekhar Azam, S. and Mariani, S. 2012 *Dual estimation of partially observed nonlinear structural systems: A particle filter approach.* Mechanics Research Communications 46, 54–61.

Simultaneous Empirical Interpolation and Reduced Basis method for non-linear problems

Christophe Prud'homme
Université de Strasbourg 7 rue René Descartes, 67084 - Strasbourg France
christophe.prudhomme@cemosis.fr

Cécile Daversin
Université de Strasbourg
7 rue René Descartes, 67084 - Strasbourg France
daversin@math.unistra.fr

In this talk, we will focus on the reduced basis methodology in the context of non-linear and non-affinely parametrized partial differential equations in which affine decomposition necessary for the reduced basis methodology are not obtained. To deal with this issue, it is now standard to apply the Empirical Interpolation Method (EIM) methodology [1, 4] before deploying the Reduced Basis (RB) methodology. The EIM building step can be costly and require many (hundreds) finite element solutions when the terms are non-linear that forbids its application to large non-linear problems.

In this talk, we will introduce a Simultaneous EIM Reduced basis algorithm (SER) [2] based on the use of reduced basis approximations into the EIM building step. Enjoying the efficiency offered by reduced basis approximation, this method provides a huge computational gain and can require as little as $N + 1$ finite element solves where N is the dimension of the RB approximation and allows to recover the approximation properties when using the standard approach.

We will start this talk with a brief overview of the EIM and RB methodologies applied to non-linear problems. The identification of the main issue, discussing the changes to be made in the EIM offline step for such problems will then introduce the SER method detailed in the first part of the talk with some of its variants. The second part of the talk will first illustrate our method with results obtained on a benchmark introduced in [4]. We will then present its performances for large scale problems it is designed for, through a 3D non-linear multi-physics reduced model used in high field magnet optimization context introduced in [3].

The SER method is now available in the generic and seamlessly parallel reduced basis framework of the opensource library Feel++ (Finite Element method Embedded Language in C++, `http://www.feelpp.org`). An online demonstrations will be done.

References

[1] M. Barrault, Y. Maday, N. C. Nguyen, and A. Patera. An empirical interpolation method: application to efficient reduced-basis discretization of partial differential equations. *Comptes Rendus Mathematique*, 339(9):667–672, 2004.

[2] C. Daversin and C. Prud'homme. Simultaneous empirical interpolation and reduced basis method for non-linear problems. *Comptes Rendus Mathematique*, 353(12):1105 – 1109, 2015.

[3] C. Daversin, S. Veys, C. Trophime, and C. Prud'Homme. A reduced basis framework: Application to large scale nonlinear multi-physics problems. *Esaim Proc.*, 43:225–254, Dec. 2013.

[4] M. Grepl, Y. Maday, N. C. Nguyen, and A. Patera. Efficient reduced-basis treatment of nonaffine and nonlinear partial differential equations. *ESAIM: Mathematical Modelling and Numerical Analysis*, 41(03):575–605, 2007.

Multi-Index Stochastic Collocation (MISC) for random elliptic PDEs

Lorenzo Tamellini
IMATI-CNR
via Ferrata 1, 27100 - Pavia Italy
tamellini@imati.cnr.it

Abdul-Lateef Haji-Ali
King Abdullah University of Science and Technology
Thuwal 23955-6900 - Saudi Arabia
abdullateef.hajiali@kaust.edu.sa

Fabio Nobile
École Polytechnique Fédérale de Lausanne
EPFL-SB-MATHICSE-CSQI, Building Math, Station 8, CH-1015 - Lausanne Switzerland
fabio.nobile@epfl.ch

Raul Tempone
King Abdullah University of Science and Technology
Thuwal 23955-6900 - Saudi Arabia
raul.tempone@kaust.edu.sa

In this talk we describe the Multi-Index Stochastic Collocation method (MISC) for computing statistics of the solution of a PDE with random data. MISC is a combination technique based on mixed differences of spatial approximations and quadratures over the space of random data; in other words, the approximation is computed as a linear combination of several smaller approximation computed over relatively coarse grids in space and probability. We propose an optimization procedure to select the most effective mixed differences to include in the MISC estimator: such optimization is a crucial step and allows us to build a method that, provided with sufficient solution regularity, is potentially more effective than other multi-level collocation methods already available in literature.
We provide a complexity analysis both in the case of a finite and an infinite number of random variables, showing that in the optimal case the convergence rate of MISC is only dictated by the convergence of the deterministic solver applied to a one dimensional problem. We show the effectiveness of MISC with some computational tests, comparing it with other related methods available in the literature, such as the Multi-Index and Multilevel Monte Carlo, Multilevel Stochastic Collocation, Quasi Optimal Stochastic Collocation and Sparse Composite Collocation methods.

Multi space reduced basis (MSRB) preconditioners for large-scale parametrized PDEs

Niccolò Dal Santo
CMCS-MATHICSE-SB École Polytechnique Fédérale de Lausanne
Station 8, CH-1015 Lausanne, Switzerland
niccolo.dalsanto@epfl.ch

Simone Deparis
CMCS-MATHICSE-SB École Polytechnique Fédérale de Lausanne
Station 8, CH-1015 Lausanne, Switzerland
simone.deparis@epfl.ch

Andrea Manzoni
CMCS-MATHICSE-SB École Polytechnique Fédérale de Lausanne
Station 8, CH-1015 Lausanne, Switzerland
andrea.manzoni@epfl.ch

Alfio Quarteroni
CMCS-MATHICSE-SB École Polytechnique Fédérale de Lausanne
Station 8, CH-1015 Lausanne, Switzerland
alfio.quarteroni@epfl.ch

In this talk we present a new 2-level preconditioner for the efficient solution of large-scale linear systems arising from the discretization of parametrized PDEs. Our preconditioner combines multiplicatively a reduced basis (RB) coarse solver and a nonsingular preconditioner, such as 1-level Additive Schwarz, Gauss-Seidel or Jacobi preconditioner. The proposed technique hinges upon the construction of a new Multi Space Reduced Basis (MSRB) method, where a reduced space is built through proper orthogonal decomposition at each iteration of the Richardson or the flexible GMRES method used to solve the large-scale linear system. As a matter of fact, each reduced space is suited to solve a particular iteration and aims at fixing the scales that have not been treated by previous iterations and the fine preconditioner yet. Not only, the RB error decays exponentially fast for each space, thus yielding to very small (compared to the dimension of the original system) reduced spaces. Since the RB accuracies obtained for each space affect the overall convergence of the iterative method in a multiplicative way, a very accurate solution of the large-scale system can be computed in very few (order than 10) iterations. Numerical tests have been carried out to evaluate the performance of the preconditioner in different large-scale modeling settings related to parametrized advection-diffusion-reaction equations, up to millions of degrees of freedom, and compared with the current state-of-art algebraic multigrid preconditioners.

Design-space Dimensionality Reduction in Hydrodynamic Shape Optimization by Generalized Karhunen-Loève Expansion

Andrea Serani
CNR-INSEAN, Natl. Research Council-Marine Technology Research Inst.
via di Vallerano 139 - 00128 Rome, Italy
andrea.serani@insean.cnr.it

Cecilia Leotardi
CNR-INSEAN, Natl. Research Council-Marine Technology Research Inst.
via di Vallerano 139 - 00128 Rome, Italy
cecilia.leotardi@cnr.it

Emilio F. Campana
CNR-INSEAN, Natl. Research Council-Marine Technology Research Inst.
via di Vallerano 139 - 00128 Rome, Italy
emiliofortunato.campana@cnr.it

Matteo Diez
CNR-INSEAN, Natl. Research Council-Marine Technology Research Inst.
via di Vallerano 139 - 00128 Rome, Italy
matteo.diez@cnr.it

Frederick Stern
IIHR-Hydroscience & Engineering, The University of Iowa
Iowa City, IA 52242, USA
frederick.stern@uiowa.edu

The design of aerial, marine, and ground vehicles involves a number of different and often conflicting disciplines, requiring accurate analyses and complex decision making methodologies. In the last decades, the design process has been substantially modified by the availability of high-fidelity computer simulation tools and high performance computing systems. The design paradigm has shifted from the *build-and-test* approach to more efficient, effective, and versatile *simulation-based design* methodologies. The integration of optimization algorithms with computer simulations has led to automatic simulation-based design *optimization* (SBDO) procedures, with the aim of assisting and possibly guiding the designer in the the decision making process of complex engineering applications.
SBDO has been widely applied to aerospace [6], naval [5], and automotive [4] applications, where the shape design is of primary importance for the vehicle performance (e.g., aerodynamic, aeroelasticity, flight mechanics, hydrodynamics, seakeeping, structures, heat transfer). In this context, an automated SBDO needs to integrate (i) simulation tools (for fluids, structures, etc.) and (ii) optimization algorithms with (iii) geometry modification and automatic meshing algorithms (see the right block in Fig. 1). To obtain an automated process this three fundamental elements have to be coupled together in a robust and

efficient way.

High-fidelity simulations based on PDE are required to achieve accurate solutions

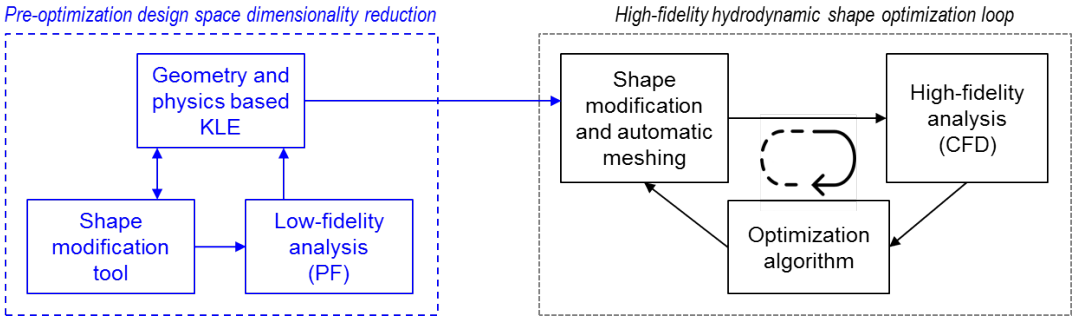


Figure 1: SBDO scheme for hydrodynamic shape optimization, including pre-optimization design-space dimensionality reduction [3]

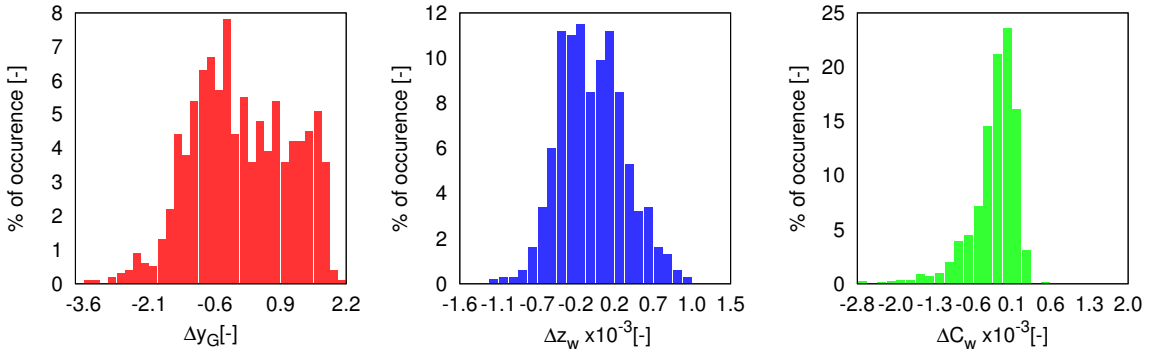
and drive effectively the optimization algorithm towards the (possibly global) optimum. Furthermore, real world applications are affected by uncertainty and therefore require an accurate modeling of environmental and operating conditions and the solution of an uncertainty quantification problem within the optimization loop, in order to achieve robust design solutions. Despite the increased computational power of HPC systems and efficiency of numerical algorithms, high-fidelity SBDO for deterministic and/or stochastic shape optimization still remains a challenging process, from theoretical, algorithmic, and technological viewpoints. One of the most complex challenges is how to deal with high-dimensional, large design spaces, especially when computationally-expensive black-box functions are used for the performance analysis. Potential design improvements significantly depend on dimension and extension of the design space: high dimension and variability spaces are more difficult and expensive to explore but, at the same time, potentially allow for larger improvements. The assessment and breakdown of the design-space variability is therefore a key element for the success of the SBDO.

Some recent research focused on design-space dimensionality reduction for efficient uncertainty quantification and optimization procedures. In [7], the Karhunen-Loève expansion (KLE, also known as proper orthogonal decomposition, POD) is used for representing distributed geometrical uncertainties and building a reduced-order spatial model for uncertainty quantification. In [1], a quantitative approach based on the KLE has been formulated for a pre-optimization assessment of the shape modification variability and the definition of a reduced-dimensionality global model of the shape modification. The method has been successfully applied for deterministic [8] and stochastic [2] hydrodynamic optimizaiton. Lately, [3] extended the KLE formulation for dimensionality reduction to combined geometry and physics based design variability.

The objective of the current work is to present recent developments in the application of a generalized KLE formulation to design-space dimensionality reduction in hydrodynamic shape optimization. The method proposed provides the breakdown of geometry and physics based design variability, as lately developed and presented in [3]. The approach is schematized in Fig. 1, where the left box includes the elements of the pre-optimization design-space dimensionality reduction. Design spaces are assessed in terms of eigenmodes and eigenvalues of an integral operator. The eigenvalues equal the design variability (variance) associated to the corresponding eigenmodes, which are used as a basis to build a reduced-dimensionality representation of the shape modification. Details of equations and numerical implementation are given in [1, 3].

The method is demonstrated for the optimization in calm water of the DTMB 5415, an early and open-to-public version of the DDG-51 (an USS Arleigh Burke-class destroyer). The geometry of the hull is modified to reduce the resistance at Fr=0.25. The physics taken into account includes the wave elevation and the wave resistance coefficient, evaluated by the sake of design-space dimensionality reduction by a low fidelity solver (potential flow).

Figure 2 shows the variability associated to a 27-dimensional design space, obtained



(a) Geometry (b) Wave elevation (c) Wave resistance coefficient

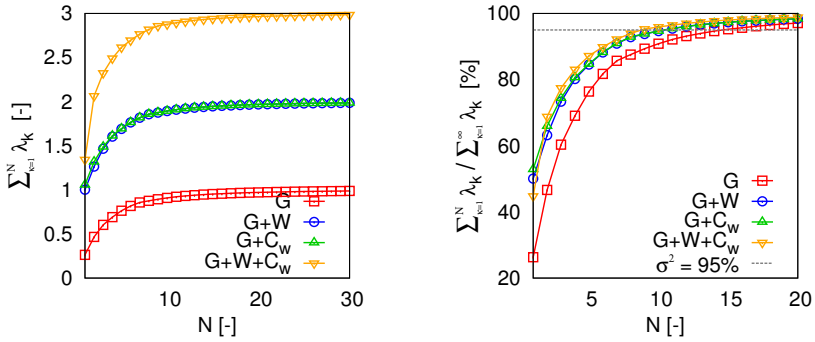
Figure 2: Geometry and physics based design variability for the DTMB 5415 in calm water at Fr=0.25, using $S = 1000$ random designs [3]

by a global modification of the 3D space that embeds the DTMB 5415 [8]. Specifically, 1000 random designs were produced and the corresponding histogram analysis is shown in Fig. 2 (a), (b) and (c), for a point of the hull (geometry variation), a point of the free surface (variation of the wave elevation), and finally the variation of the wave resistance coefficient. The design-space dimensionality reduction is performed considering four vector spaces, formed by: geometry only (G), geometry and wave elevation (G+W), geometry and wave resistance coefficient (G+C_W), and finally geometry, wave elevation, and wave resistance coefficient (G+W+C_W). Figures 3 (a) and (b) show, respectively, the absolute and relative design variability (in terms of cumulative sum of eigenvalues provided by KLE) associated to a dimensionality-reduced space of dimension N. Using G, the 95% of the original design variability is achieved by $N = 15$. Extending to physics based analysis, a number of design variables equal to $N = 11$, 11, and 9 is required, using G+W, G+C_W, and G+W+C_W, respectively. Figure 4 (a), (b), (c), and (d) show, for each space, the basis function (geometry domain) that resolves the largest design variability.

The current results show how the combined geometry and physics based analysis improves the effectiveness of the design-space dimensionality reduction, allowing for a more efficient definition of the design space for hydrodynamic shape optimization.

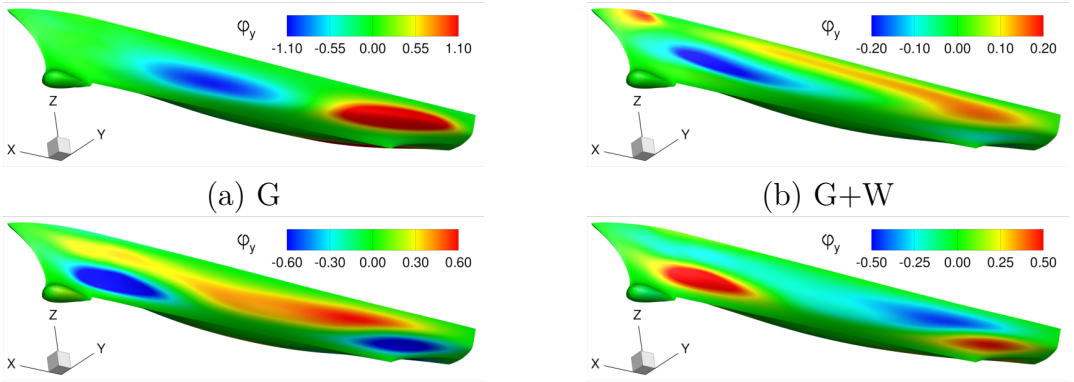
Acknowledgements.

The research is supported by the Office of Naval Research (ONR), NICOP grant N62909-15-1-2016 and grant N00014-14-1-0195, administered by Dr. Woei-Min Lin and Dr. Ki-Han Kim, and by the Italian Flagship Project RITMARE, coordinated by the Italian National Research Council and founded by the Italian Ministry of Education, and conducted in collaboration with NATO STO Task Group AVT-204, formed to "Assess the Ability to Optimize Hull Forms of Sea Vehicles for Best Performance in a Sea Environment."



(a) Absolute values (b) Relative values

Figure 3: Design variability (variance) retained by a reduced-dimensionality space of dimension N [3]



(a) G (b) G+W

(c) G+C$_W$ (d) G+W+C$_W$

Figure 4: Basis functions (geometry domain) resolving the largest design variability, for each design space [3]

References

[1] Diez M., Campana E.F. and Stern F. 2015 *Design-space dimensionality reduction in shape optimization by Karhunen–Loéve expansion.* Computer Methods in Applied Mechanics and Engineering, Vol. 283, pp. 1525-1544.

[2] Diez M., Campana E.F. and Stern F. 2015 *Development and evaluation of hull-form stochastic optimization methods for resistance and operability.* FAST 2015 - 13th International Conference on Fast Sea Transportation, Washington DC, USA, 1-4 September 2015.

[3] Diez M., Serani A., Stern F. and Campana, E.F. 2016 *Combined Geometry and Physics Based Method for Design-space Dimensionality Reduction in Hydrodynamic Shape Optimization.* Proceedings of 31th Symposium on Naval Hydrodynamics, Monterey CA, USA, 11-16 September 2016.

[4] Hojjat, M., Stavropoulou, E., and Bletzinger, K.U. 2014 *The Vertex Morphing method for node-based shape optimization.* Comput. Methods Appl. Mech. Engrg., Vol. 268, pp. 494–513.

[5] Kandasamy, M., Peri, D., Tahara, Y., Wilson, W., Miozzi, M., Georgiev, S., Milanov, E., Campana, E. F., and Stern, F. 2013 *Simulation-based design optimization of waterjet propelled Delft catamaran.* International Shipbuilding Progress, Vol. 60(1), pp. 277–308.

[6] Kotinis, M. and Kulkarni, A. 2012 *Multi-objective shape optimization of transonic airfoil sections using swarm intelligence and surrogate models.* Structural and Multidisciplinary Optimization, Vol. 45(5), pp. 747–758.

[7] Schillings, C., Schmidt, S., and Schulz, V. 2011 *Efficient shape optimization for certain and uncertain aerodynamic design.* Computers & Fluids, Vol. 46(1), pp. 78–87.

[8] Serani A., Fasano G., Liuzzi G., Lucidi S., Iemma U., Campana E.F., Stern F. and Diez M. 2016 *Ship hydrodynamic optimization by local hybridization of deterministic derivative-free global algorithms.* Applied Ocean Research, Elsevier, in press.

Large-scale and Data-driven PDE problems: Uncertainty Quantification & Reduced Order Modeling - Part III

PROPOSERS

Andrea Manzoni
Ecole Polytechnique Fédérale de Lausanne (EPFL)
av. Piccard, Station 8, CH-1015 - Lausanne, Switzerland
andrea.manzoni@epfl.ch

Lorenzo Tamellini
Istituto di Matematica Applicata e Tecnologie Informatiche (IMATI) - CNR
Via Ferrata 1, 27100 - Pavia, Italy
tamellini@imati.cnr.it

SPEAKERS

Sandra Pieraccini
Dip. Matematica, Politecnico di Torino
sandra.pieraccini@polito.it

James Irving
Institute of Earth Sciences, University of Lausanne
james.irving@unil.ch

Ivo Colombo
Dip. Ing. Civile e Ambientale, Politecnico di Milano
ivo.colombo@polimi.it

Alessio Spantini
Dept. of Aeronautics and Astronautics, MIT
spantini@mit.edu

Loïc Giraldi
Applied Math. and Comp. Science, KAUST
loic.girandi@kaust.edu.sa

Daniele Bigoni
Dept. of Aeronautics and Astronautics, MIT
dabi@mit.edu

A growing number of applications in engineering requires to merge mathematical models built on partial differential equations and complex data (possibly high-dimensional and/or affected by uncertainty) in order to perform tasks such as driving a system to a desired target, ensuring minimal operational risk, identifying its unknown features or exploring efficiently different scenarios. Data assimilation, uncertainty quantification, PDE-constrained optimization and inverse problems are therefore becoming more and more the mainstays of modern computational science. However, while recent advances

in reduced order modeling and uncertainty quantification techniques increasingly allow to successfully tackle large-scale problems using computationally tenable algorithms, several outstanding theoretical and algorithmical challenges remain. The purpose of this minisymposium is to bring together researchers who are active in the above-mentioned fields, to present novel and promising methods, and to discuss future trends for research.

Uncertainty quantification in discrete fracture networks with stochastic parameters

Sandra Pieraccini
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
sandra.pieraccini@polito.it

Stefano Berrone
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
stefano.berrone@polito.it

Claudio Canuto
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
claudio.canuto@polito.it

Stefano Scialò
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
stefano.scialo@polito.it

We consider the framework of subsurface flow simulation in fractured media modelled by the so-called Discrete Fracture Network (DFN) approach. Within this model, the fractured medium is described as an (impervious) rock matrix crossed by fractures, represented as planar polygons, with various orientation in space, intersecting each other along segments called *traces*. The flow occurs along fractures, and flux exchange takes place across traces. The flow on the overall network is driven by the Darcy law, locally imposed on fractures; these local problems are coupled by suitable matching conditions ensuring flux balance at the fractures intersections.
Since deterministic data about the underground are not fully available, networks are generated starting from probabilistic distributions for both hydro-geological properties (such as fracture transmissivity) and geometrical features (orientation in the 3D space, position, dimension, and aspect ratio). The issue of quantifying the influence of these stochastic parameters on the output of DFN models is therefore of crucial importance, especially in applications related to safety investigation of underground exploitation processes, such as for example geological storage, aquifer monitoring, oil & gas enhanced production. An example of realistic test case under investigation is depicted in Figure 1, representing a network in which an injection well and an extraction well are connected, by means of a fracture network, to a large fault. The investigation here can be related to the monitoring of the dispersion of a pollutant injected in the network.
Due to the complexity of each simulation, a *non-intrusive* approach [6] is recommended, in such a way that the solver acts as a *black-box*. Furthermore, the high computational cost calls for the use of modern UQ techniques [1] which allow for effective computation

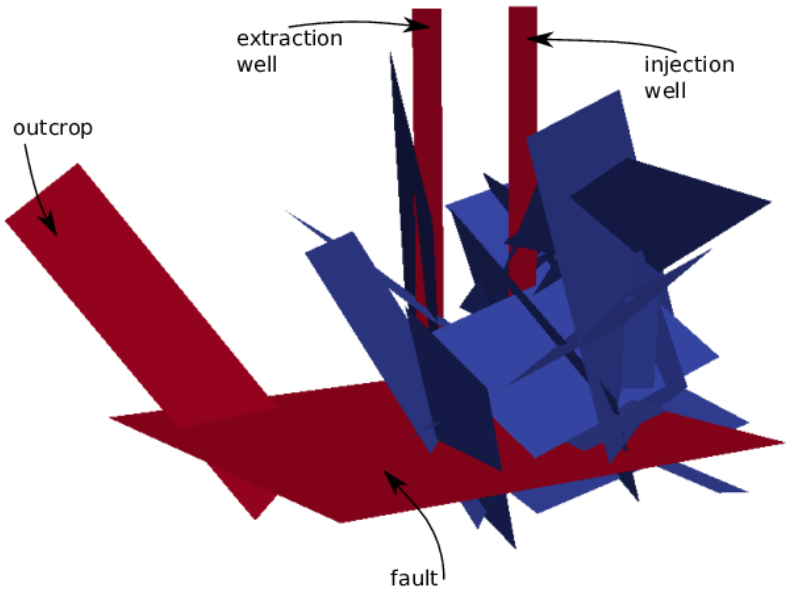


Figure 1: Example of DFN

of statistics of interest with a moderate number of calls to the black-box.
Within this context, we will consider stationary problems with stochastic geometrical parameters, and non-stationary problems with deterministic geometry and stochastic hydro-geological parameters (see, e.g., Figure 2, in which the dispersion of a pollutant in the network is monitored).

In both the described cases, we will address the problem of computing statistics of

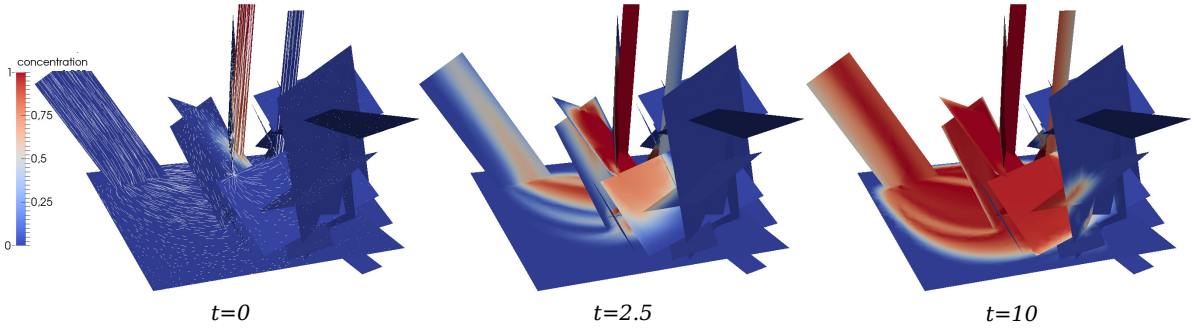


Figure 2: Pollutant dispersion

the quantity of interest by means of suitable, effective UQ strategies. In particular, collocation strategies (using sparse grids [4] in the stochastic multi-dimensional case) and the Multi-level Monte Carlo method [5] will be considered, obtaining good approximations of the first and second order moments of the quantity of interest. As an example, we depict in Figure 3 the behaviour of the errors obtained in computing the expected value of the overall flux flowing through a given network, in which the fracture dimensions are stochastically generated.

In all the considered cases, of crucial importance will be the robustness [2, 3] of the underlying solver, which should be able to tackle whatever complex geometrical configuration is stochastically generated.

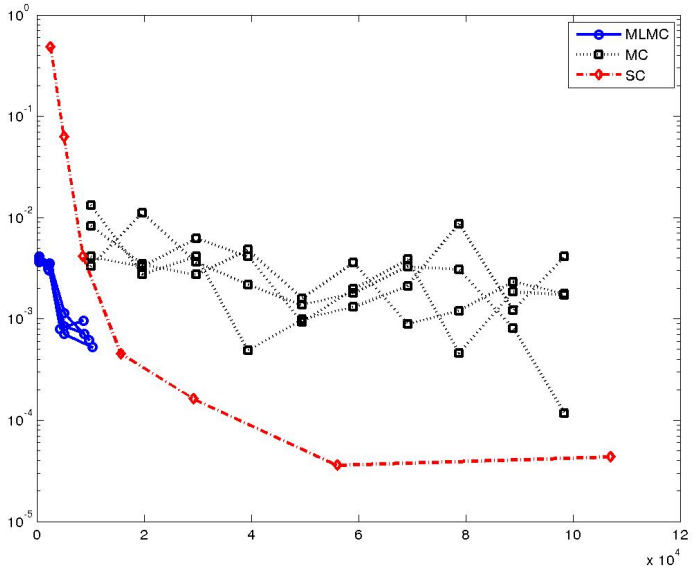


Figure 3: Approximation of the expected value of the flux flowing through a DFN with stochastic geometry: errors versus computational cost with Multi-level Monte Carlo (MLMC), standard Monte Carlo (MC), multi-element stochastic collocation (SC)

References

[1] Berrone, S., Canuto, C., Pieraccini, S. and Scialò, S. 2015 *Uncertainty quantification in Discrete Fracture Network models: stochastic fracture transmissivity.* Computer & Mathematics with Applications 70, 603–623.

[2] Berrone, S., Pieraccini, S. and Scialò, S. 2014 *An optimization approach for large scale simulations of discrete fracture network flows.* Journal of Computational Physics 256, 838–853.

[3] Berrone, S., Pieraccini, S., Scialò, S. and Vicini, F. 2015 *A parallel solver for large scale DFN flow simulations.* SIAM J. Sci. Comput. 37, C285–C306.

[4] Bungartz, H.-J. and Griebel, M. 2004 *Sparse grids.* Acta Numerica 13, 147–269.

[5] Giles, M. B. 2008 *Multi-level Monte Carlo path simulation.* Operations Research 56, 607–617

[6] Le Maître, O. P. and Knio, O. M. 2010 *Spectral methods for uncertainty quantification. With applications to computational fluid dynamics.* Springer.

Addressing the issue of model error in Bayesian solutions to near-surface geophysical inverse problems

James Irving
University of Lausanne
1015 Lausanne, Switzerland
james.irving@unil.ch

Corinna Koepke
University of Lausanne
1015 Lausanne, Switzerland
corinna.koepke@unil.ch

Delphine Roubinet
University of Lausanne
1015 Lausanne, Switzerland
delphine.roubinet@unil.ch

1 Introduction

Geophysical methods have gained much interest in hydrology because of their ability to provide estimates of the spatial distribution of subsurface properties at a scale that is often relevant to key hydrological processes. Because of an increased desire to quantify uncertainty in hydrological predictions, many of the corresponding inverse problems have recently been posed within a Bayesian framework. With the Bayesian approach, it is often necessary to make significant approximations to the hydrological and geophysical forward models such that stochastic sampling from the posterior distribution, for example using Markov-chain-Monte-Carlo (MCMC) methods, is computationally feasible. These approximations lead to model errors which are notoriously difficult to characterize for real-world geophysical problems as they are often highly non-Gaussian, strongly correlated, and spatially and temporally variable. Here we present a practical approach for model error identification and removal that is based on the idea that model error can sometimes be separated from parameter and data uncertainties through learning about its behaviour from stochastic realizations. We apply this approach to the problem of estimating subsurface unsaturated hydraulic parameters from zero-offset-profile crosshole ground-penetrating radar data.

2 Bayesian geophysical inversion

Consider the general forward problem linking a set of N measured or observed data $\mathbf{d}_{obs} \in \mathbb{R}^N$ to a set of M subsurface model parameters of interest $\mathbf{m}_{true} \in \mathbb{R}^M$:

$$\mathbf{d}_{obs} = \mathcal{F}(\mathbf{m}_{true}) + \mathbf{e}_d, \tag{1}$$

where forward operator $\mathcal{F} : \mathbb{R}^M \rightarrow \mathbb{R}^N$ contains the physics and geometry of the measurements and $\mathbf{e}_d$ is vector of data measurement errors. Within a probabilistic framework, the corresponding inverse problem can be formulated using Bayes' theorem, whereby an initial prior state of information for the model parameters $\rho(\mathbf{m})$ is updated into a more refined posterior state of knowledge $\sigma(\mathbf{m})$ based on the available data [1]. That is,

$$\sigma(\mathbf{m}) = k\, L(\mathbf{m})\, \rho(\mathbf{m}), \tag{2}$$

where k is a normalization constant and $L(\mathbf{m})$ is the likelihood function. Assuming that (i) the underlying physics is completely known and considered in the inverse problem, and (ii) the data measurement errors are independent and identically normally distributed having mean zero and standard deviation s_d, $L(\mathbf{m})$ has the simple multi-Gaussian form

$$L(\mathbf{m}) = \frac{1}{(2\pi s_d^2)^{N/2}} \exp\left[-\frac{||\mathbf{r}(\mathbf{m})||^2}{2s_d^2}\right], \tag{3}$$

where $\mathbf{r}(\mathbf{m})$ is the residual or difference between the observed data and those predicted for some model parameter set $\mathbf{m}$ using $\mathcal{F}$. The latter quantity is given by

$$\begin{aligned} \mathbf{r}(\mathbf{m}) &= \mathbf{d}_{obs} - \mathbf{d}_{pred} \\ &= \underbrace{\mathcal{F}(\mathbf{m}_{true}) - \mathcal{F}(\mathbf{m})}_{\text{parameter error}} + \underbrace{\mathbf{e}_d}_{\text{data error}}, \end{aligned} \tag{4}$$

where $\mathbf{d}_{pred}$ denotes the predicted data.

3 Dealing with model error

Likelihood equation (3) is perfectly theoretically valid for the case where the only contribution to the difference between the observed and predicted data, when considering the correct set of model parameters $\mathbf{m}_{true}$, is a set of Gaussian data measurement errors having known standard deviation s_d. Indeed, MCMC algorithms based on equations (2) through (4), or slight variants thereof, have been used to quantify uncertainty for a wide range of geophysical and hydrological problems under the implicit assumption that the latter condition is satisfied. In most cases, however, the forward operator considered in such inversions is either not fully known and/or it employs approximate or surrogate physics in order to make the MCMC procedure computationally tractable. As a result, the residual more commonly takes the form

$$\begin{aligned} \mathbf{r}(\mathbf{m}) &= \mathcal{F}(\mathbf{m}_{true}) - \hat{\mathcal{F}}(\mathbf{m}) + \mathbf{e}_d \\ &= \underbrace{\mathcal{F}(\mathbf{m}_{true}) - \mathcal{F}(\mathbf{m})}_{\text{parameter error}} + \underbrace{\mathcal{F}(\mathbf{m}) - \hat{\mathcal{F}}(\mathbf{m})}_{\text{model error}} + \underbrace{\mathbf{e}_d}_{\text{data error}}, \end{aligned} \tag{5}$$

where $\hat{\mathcal{F}}$ is the incorrect or approximate forward operator. The presence of an additional model error term in equation (5) as compared with equation (4), which is commonly of large magnitude, strongly correlated, and highly non-Gaussian, makes use of a Gaussian likelihood expression troublesome. In particular, it means that (i) the residual will not necessarily be minimized when $\mathbf{m} = \mathbf{m}_{true}$, implying posterior parameter bias; and (ii) feasible model parameter sets may have an extremely low likelihood when considering realistic levels of data error. Although simple and arbitrary inflation of s_d can be used to broaden the Gaussian likelihood and reduce the latter issue, it cannot address the

former and be viewed as an effective solution for obtaining reliable posterior uncertainty estimates.

For many practical problems where approximate forward operators are employed to make MCMC sampling of the Bayesian posterior distribution computationally feasible, the model error term in equation (5) may be too complicated to characterize analytically through construction of an error model. For these reasons, we consider here a learning-based approach to *identify* and then subtract the model error from $\mathbf{r}(\mathbf{m})$ before determination of the likelihood in MCMC. The overall idea is that a small number of model error training realizations, computed for random model parameter sets using the full and approximate forward operators, can be used for this purpose at significantly lower computational cost than considering the full physics forward operator directly in the MCMC procedure. Our approach can be summarized as follows:

1. Generate k random sets of model parameters $\{\mathbf{m}_1, ..., \mathbf{m}_k\}$ by drawing from the Bayesian prior distribution $\rho(\mathbf{m})$.

2. Compute the corresponding set of model error training realizations $\{\mathbf{T}_1, ..., \mathbf{T}_k\}$, where $\mathbf{T}_i = \mathcal{F}(\mathbf{m}_i) - \hat{\mathcal{F}}(\mathbf{m}_i)$.

3. Perform principal component analysis (PCA) on the training realizations $\{\mathbf{T}_1, ..., \mathbf{T}_k\}$ in order to obtain a sparse orthonormal basis $\mathbf{B} = [\mathbf{b}_1, ..., \mathbf{b}_b]$ for the model error, where the number of basis vectors b is chosen such that $\mathbf{B}$ captures some high percentage of the variance of the realizations, but has minimal ability to capture contributions to the residual that do not resemble model error such as data measurement uncertainties.

4. For each set of model parameters $\mathbf{m}'$ tested within MCMC, calculate the best least-squares approximation of the residual $\mathbf{r}(\mathbf{m}') = \mathbf{d}_{obs} - \hat{\mathcal{F}}(\mathbf{m}')$ using the model error basis, obtained using $\mathbf{B}\,\mathbf{B}^T\mathbf{r}(\mathbf{m}')$, and remove this result from the residual. This yields the remainder

$$\mathbf{R}(\mathbf{m}') = \mathbf{r}(\mathbf{m}') - \mathbf{B}\,\mathbf{B}^T\mathbf{r}(\mathbf{m}') \tag{6}$$

5. Use $\mathbf{R}(\mathbf{m}')$ to determine $L(\mathbf{m}')$ within MCMC.

References

[1] Tarantola, A. 2005 *Inverse Problem Theory and Methods for Model Parameter Identification.* SIAM.

Uncertainty Quantification for Compaction Modeling in Stratified Sedimentary Basins

Ivo Colombo
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
ivo.colombo@polimi.it

Giovanni Michele Porta
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
giovanni.porta@polimi.it

Lorenzo Tamellini
IMATI-CNR
Via Ferrata, 1 27100 - Pavia Italy
tamellini@imati.cnr.it

Anna Scotti
Politecnico di Milano
Via Bonardi, 9 20133 - Milano Italy
anna.scotti@polimi.it

Fabio Nobile
École Polytechnique Fédérale de Lausanne
EPFL-SB-MATHICSE-CSQI, Building Math, Station 8, CH-1015 - Lausanne Switzerland
fabio.nobile@epfl.ch

We employ a one-dimensional numerical model [1] to simulate the vertical compaction of sedimentary basins, characterized by alternating depositional events of sandstone and shale layers. In order to perform the uncertainty quantification analysis in an efficient way, we adopt an approach based on: (i) forward modeling of fluid flow and compaction along time and (ii) application of a model-complexity reduction technique based on sparse-grids approximation. Our technique thus relies on a polynomial surrogate model, which approximates the full compaction model, originally expressed as a coupled system of nonlinear partial differential equations. The surrogate model solution proposed in [1] is obtained following three steps: (a) selection of uncertain model parameters and their range of variability, (b) efficient sampling of the parameter space through a sparse grid technique and (c) interpolation of the model responses on the sparse grid at each depth. Observe that the sparse-grid approximation can eventually be converted into a generalized Polynomial Chaos Expansion (gPCE), whose coefficients can be algebraically post-processed to obtain relevant information for the uncertainty quantification analysis, such as statistical moments and Sobol indices of the quantities of interest.
Uncertainty quantification typically requires multiple evaluations of the model outputs in the selected parameters space. In this context, the sparse-grids-based surrogate model

is a powerful tool to reduce the computational costs. However, sparse grids typically lose accuracy in the presence of model outputs which display sharp discontinuities in the parameters space. This issue becomes particularly relevant in the context of compaction modeling, as some model outputs typically assume different values depending on the properties associated with the geo-material. For example the evolution of porosity can considerably change between sand and clay sediments, due to (i) the different mechanical properties associated to the sediments and (ii) geochemical processes leading to porosity changes which selectively take place as a function of the local sediment composition (our model e.g. considers porosity reduction due to quartz cementation which may largely affect porosity only in sandstone layers). As a consequence, vertical distributions of porosity may exhibit large discontinuities at the interface between two layers characterized by different sediment compositions. Therefore, a single depth may be associated with the presence of different geo-materials, when multiple realizations are considered within the selected parameters space. As hinted above, this corresponds to a discontinuity in the input-output mapping and prevents an accurate approximation of the complete porosity vertical profile through a polynomial approach. We present a procedure to overcome this limitation, based on a suitable remapping of the realizations to a reference domain.
An application to a (synthetic) test case is illustrated. We consider a simple domain composed by five alternating layers of sandstone and shale materials. We set to a fixed value the majority of model parameters and select only three to be considered as random: the porous medium vertical compressibility for sandstone and shale, and the shale vertical permeability. The choice of this particular set of random parameters is here adopted for illustrative purposes and is grounded on the observation that these parameters strongly influence the compaction of the domain, allowing us to emphasize the overlapping of layers of different materials. The random parameters are associated with a uniform probability density function, whose range is here assigned upon relying on real field studies. We assess the robustness of our approach through a direct comparison against the full model solution in a Monte Carlo framework, and by comparing the probability density functions referred to vertical porosity distribution obtained with the full compaction model and the surrogate model. Our results show that the proposed methodology allows reproducing multimodal probability density functions, resulting from the strongly nonlinear mapping between input and output which characterizes the considered problem.

References

[1] Formaggia, L., Guadagnini, A., Imperiali, I., Lever, V., Porta, G., Riva, M., et al. 2013 *Global sensitivity analysis through polynomial chaos expansion of a basin-scale geochemical compaction model.* Computational Geosciences, 17(1), 25–42.

Goal-oriented optimal approximations of Bayesian linear inverse problems

Alessio Spantini
Massachusetts Institute of Technology
Cambridge, MA, 02139, USA
spantini@mit.edu

Tiangang Cui
Massachusetts Institute of Technology
Cambridge, MA, 02139, USA
tcui@mit.edu

Karen Willcox
Massachusetts Institute of Technology
Cambridge, MA, 02139, USA
kwillcox@mit.edu

Luis Tenorio
Colorado School of Mines
Golden, CO, 80401, USA
ltenorio@mines.edu

Youssef Marzouk
Massachusetts Institute of Technology
Cambridge, MA, 02139, USA
ymarz@mit.edu

We propose statistically optimal and computationally efficient dimensionality reduction techniques for goal-oriented Bayesian Gaussian linear inverse problems where the QoI is a linear function of the inversion parameters. In particular, we study approximations of the posterior covariance of the QoI as a low-rank negative update of the prior covariance of the QoI and prove optimality of the update with respect to the natural geodesic distance on the manifold of symmetric and positive definite matrices. We also propose approximations of the posterior mean of the QoI as a low-rank linear function of the data and prove optimality of the approximation with respect to the Bayes risk for squared-error loss weighted by the posterior precision matrix of the QoI. These optimal approximations avoid the explicit computation of the full posterior distribution of the parameters and focus entirely on directions that are well informed by the data and that are relevant to the QoI. These directions are obtained from the leading generalized eigenvectors of a suitable matrix pencil and stem from a careful balance between all the ingredients of the goal oriented inverse problem: prior information, forward model, measurement noise and ultimate goals.

Uncertainty quantification for the 2010 Chile earthquake source parameters: propagation, inference and reduction

Loïc Giraldi
King Abdullah University of Science & Technology
4700 KAUST, Thuwal, Jeddah 23955-6900, Kingdom of Saudi Arabia
loic.giraldi@kaust.edu.sa

Ibrahim Hoteit
King Abdullah University of Science & Technology
4700 KAUST, Thuwal, Jeddah 23955-6900, Kingdom of Saudi Arabia
ibrahim.hoteit@kaust.edu.sa

Omar Knio
King Abdullah University of Science & Technology
4700 KAUST, Thuwal, Jeddah 23955-6900, Kingdom of Saudi Arabia
omar.knio@kaust.edu.sa

Olivier Le Maître
Laboratoire d'Informatique pour la Mécanique et les Sciences de l'Ingénieur
Campus universitaire bât 508, Rue John von Neumann, F - 91405 Orsay cedex
olm@limsi.fr

This work focuses on the Bayesian inference of parameters associated to the Chile 2010 earthquake. The objective is to estimate the location, the orientation as well as the slip of a single fault earthquake model through the generated tsunami and the data gathered by an offshore buoy. In order to achieve this objective, we must address several difficulties concerning the computation of a surrogate model, its reduction, and the construction of a pertinent Bayesian model that can handle the limitations of the numerical solution of the forward problem and the data.
The data are provided by a single DART (Deep-ocean Assessment and Reporting of Tsunami) station, which measures the sea surface anomaly. As illustrated in Figure 1, we can see that the gauge is far away from the prior belief on the position of the earthquake, and therefore the data might not contain enough information to properly infer the properties of the earthquake. Figure 1 also shows that the stationary assumption of the noise process does not hold, and exhibits a correlation structure that has to be taken into account.
Denoting by ξ the random vector to infer, M the numerical forward model, ε the noise and Y the predicted signal at the DART buoy, we adopt the following additive model

$$Y(t) = M(t;\xi) + \varepsilon(t), \quad \forall t \in \{t_1, \ldots, t_n\}.$$

The prior distribution of ξ is supposed to be uniform while the noise is defined by a parametric Gaussian process $\varepsilon \sim \mathcal{N}(\theta_1, C_\varepsilon(\theta))$. The noise is defined as the sum of a biased independent Gaussian model and a zero-mean process with a Matérn 3/2 covariance which

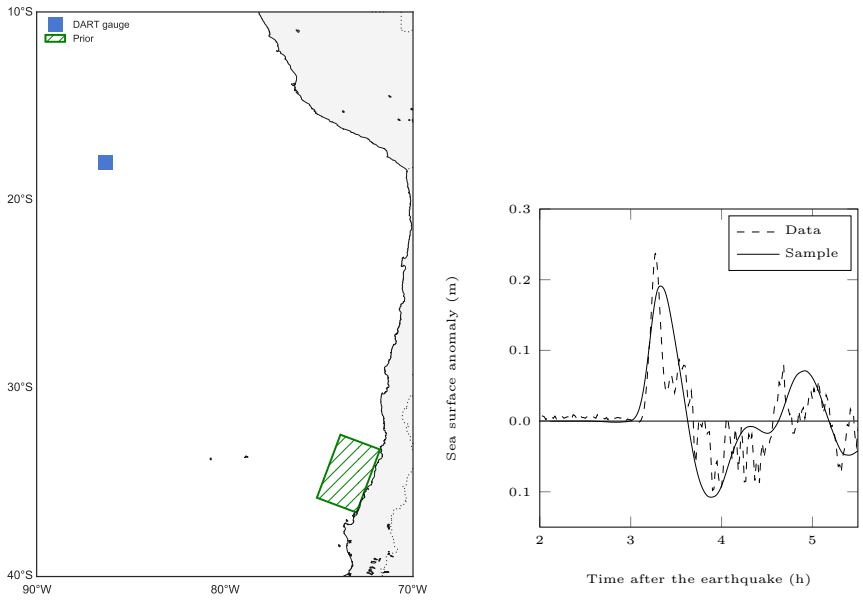


Figure 1: Left: Prior location of the earthquake and position of the DART buoy. Right: Comparison between the signal recorded by the gauge and a sample of the forward model.

captures the model error after the arrival of the tsunami at the gauge. The uniformly distributed hyperparameter θ is assumed to be independent of ξ and is also inferred from the data. The joint posterior distribution of the parameters ξ and θ is therefore given by the Bayes theorem stating that

$$p(\xi, \theta | Y = y) \propto p(Y = y | \xi, \theta),$$

since all the priors are uniform.
In order to sample from the posterior distribution, we will use the adaptive Metropolis-Hastings algorithm [2]. It is a Markov-Chain Monte-Carlo method that requires a large number of evaluations of the forward model M, which is prohibitive. Indeed, one sample of M requires us to solve the 2D shallow water equation taking into account the bathymetry variation for a relatively large time frame with the GeoClaw software [1]. An inexpensive polynomial-based surrogate model is therefore introduced in order to accelerate the inference. Since the forward M is not smooth due to different arrival times $a(\xi)$ of the waves depending on the parameter, we first introduce a suitable time transform such that

$$M(t; \xi) = M_\tau(\tau; \xi), \quad \tau = t - a(\xi).$$

As a consequence, the waves arrive at the same fictitious time $\tau = 0$ at the buoy and the model M_τ is smoother with respect to ξ than M. Given the fully tensorized Legendre polynomials $(\psi_\alpha)_{\alpha \in \mathcal{A}}$ where $\mathcal{A}$ is a finite set of multi-indices, the model is approximated by

$$M(t; \xi) \approx \sum_{\alpha \in \mathcal{A}} M_{\tau,\alpha} \left(t - \sum_{\beta \in \mathcal{A}} a_\beta \psi_\beta(\xi); \xi \right) \psi_\alpha(\xi).$$

The coefficients $(M_\alpha)_{\alpha \in \mathcal{A}}$ and $(a_\alpha)_{\alpha \in \mathcal{A}}$ are computed by L^2 projection with the non-intrusive spectral projection method [3]. The convergence of the posterior distribution is then numerically assessed using the Shannon entropy of a probability density function f defined by $H(f) = \mathbb{E}_f(-\log(f))$.

We discuss model reduction techniques which are suitable for the Bayesian framework based on the singular value decomposition (SVD). The decomposition provides the optimal space $\mathcal{V}_r$ of dimension r which minimizes the mean square error

$$\mathbb{E}\left(\|M(\xi) - P_{\mathcal{V}_r} M(\xi)\|^2\right) = \min_{\substack{\mathcal{W} \\ \dim \mathcal{W} = r}} \mathbb{E}\left(\|M(\xi) - P_{\mathcal{W}} M(\xi)\|^2\right).$$

In particular, we introduce a SVD based on the Mahalanobis distance which greatly improves the convergence of the posterior distribution with respect to the dimension of the space r. Finally, we will analyze the possibility of defining optimal subspaces dedicated to the approximation of the posterior distribution through an information gain analysis based on the Kullback-Leibler divergence. Numerical results will be presented and discussed.

References

[1] Berger, M. J., George, D. L., LeVeque, R. J., and Mandli, K. T. 2011. *The GeoClaw software for depth-averaged flows with adaptive refinement.* Advances in Water Resources, 34(9), 1195-1206.

[2] Haario, H., Saksman, E., and Tamminen, J. 2001. *An adaptive Metropolis algorithm.* Bernoulli, 223-242.

[3] Reagan, M. T., Najm, H., Ghanem, R. G., and Knio, O. M. 2003 *Uncertainty quantification in reacting-flow simulations through non-intrusive spectral projection.* Combustion and Flame 132 (3), 545–555.

Adaptive construction of measure transports, with application to Bayesian inference

Daniele Bigoni
Massachusetts Institute of Technology
77 Massachusetts Avenue; Cambridge, MA 02139 USA
dabi@mit.edu

Alessio Spantini
Massachusetts Institute of Technology
77 Massachusetts Avenue; Cambridge, MA 02139 USA
spantini@mit.edu

Youssef Marzouk
Massachusetts Institute of Technology
77 Massachusetts Avenue; Cambridge, MA 02139 USA
ymarz@mit.edu

Measure transport is a valuable tool for characterizing multivariate non-Gaussian target distributions [1, 2, 3, 4] via sampling or quadrature. This task has a broad range of applications, many of which center on statistical inference—e.g., the solution of Bayesian inverse problems, as well as filtering and smoothing in dynamical systems. The transport approach seeks a deterministic map that pushes forward a reference distribution to the target distribution of interest. An important property of this method is that it allows the parallel exploration of the target distribution and the parallel generation of independent samples. The map is constructed by minimizing the Kullback-Leibler divergence from pushforward of the reference distribution to the target distribution. This minimization problem becomes challenging in high dimensions, however, and finding an efficient parameterization of the map can become nontrivial as the target departs significantly from Gaussianity (in the case of a Gaussian reference). To tackle the first challenge, we identify and exploit several sources of sparsity in order to reduce the dimensionality of the problem [5]. To tackle the second challenge, we introduce an iterative and adaptive approach that analyzes the first variation of the minimization problem to identify *a posteriori* refinement directions at negligible additional cost. These methods will be demonstrated on inference problems arising in spatial statistics and differential equations.

References

[1] Moselhy, T. and Marzouk, Y. M. (2012). *Bayesian inference with optimal maps.* Journal of Computational Physics, 231(23): 7815–7850. http://doi.org/10.1016/j.jcp.2012.07.022

[2] Parno, M. and Marzouk, Y. M. (2015). *Transport map accelerated Markov chain Monte Carlo.* arXiv:1412.5492

[3] Parno, M., Moselhy, T., and Marzouk, Y. M. (2015). *A multiscale strategy for Bayesian inference using transport maps*. arXiv:1507.07024

[4] Marzouk, Y. M., Moselhy, T., Parno, M., and Spantini, A. (2016). *An introduction to sampling via measure transport*. In *Handbook of Uncertainty Quantification*, D. Higdon, R. Ghanem, H. Owhadi, eds. Springer. arXiv:1602.05023

[5] Spantini, A., Bigoni, D., Marzouk, Y. M. (in preparation). *Measure transport, variational inference, and low-dimensional maps*.

Advances in HPC for Geophysical Applications - Part I

PROPOSERS

Giovanni Tumolo
The Abdus Salam International Centre for Theoretical Physics and OGS
Strada Costiera, 11 34151 - Trieste Italy
gtumolo@ictp.it

Paolo Crosetto
C2SM/CSCS-ETHZ, Zürich
Via Trevano, 100 6900 - Lugano Switzerland
paolo.crosetto@usys.ethz.ch

SPEAKERS

Dimitri Komatitsch (keynote)
Laboratory of Mechanics and Acoustics, CNRS/University of Aix-Marseille, France
komatitsch@lma.cnrs-mrs.fr

Carlo Cavazzoni
SCAI (SuperComputing Applications and Innovation) department - CINECA, Bologna, Italy
c.cavazzoni@cineca.it

Matteo Cerminara
INGV Istituto Nazionale di Geofisica e Vulcanologia, Pisa, Italy
matteo.cerminara@ingv.it

Chaulio Ferreira
Technical University of Munich
chaulio.ferreira@tum.de

Silvia Mocavero
Advanced Scientific Computing Division, Centro Euro-Mediterraneo sui Cambiamenti Climatici (CMCC), Lecce, Italy
silvia.mocavero@cmcc.it

In order to effectively address the complex multidisciplinary problems arising in geophysics, a wide variety of cross competences is required. Numerical methods are used to solve complex coupled physical models on state of the art supercomputers. In particular the efficient use of supercomputing facilities is of utmost importance for most of the geophysical applications, and the detailed knowledge of the recent trends in supercomputing hardware might affect the choice of the numerical technique employed and of its implementation. For these reasons a close interaction between domain scientists, experts in numerics, and High Performance Computing experts is highly beneficial. With this minisymposium we aim at gathering experts from the three aforementioned fields, namely geophysical science, numerical methods, and HPC, in order to facilitate interactions and to enhance collaborations across the domains.

Remark Dimitri Komatitsch is our key-note speaker, therefore we allocated a double slot for him.

High-frequency modeling and imaging based on acoustic waves and HPC in geosciences and non-destructive testing

Dimitri Komatitsch
Laboratory of Mechanics and Acoustics, CNRS,
8 rue Enrico Fermi, 13453 - Marseille, France
komatitsch@lma.cnrs-mrs.fr

Owing to the progress of high-performance computing resources and numerical simulation techniques, waveform inversion approaches nowadays become a viable alternative to classical ray-based tomographic approaches.
Exploiting full waveforms in seismic tomography requires an efficient and precise method to solve the elastic wave equation in 3D inhomogeneous media. Since resolution of waveform inversion is limited by the seismic wavelength, it is crucial to exploit short-period teleseismic waves recorded by dense regional arrays. However, modelling the propagation of short-period body waves in heterogeneous media is still very challenging, even on the largest modern supercomputers. For this reason, we have developed a hybrid method that couples a global wave propagation method in a 1D Earth to a 3D spectral-element method in a regional domain. This hybrid method restricts the costly 3D computations to inside the regional domain, which dramatically decreases the computational cost. It thus allows us to compute teleseismic wavefields down to 1s period, thus accounting for the complexities that affect the propagation of seismic waves in the regional domain.
We thus present the first application of this new waveform inversion approach to broadband data coming from two dense transects deployed during the PYROPE experiment across the Pyrenees Mountains [1]. More generally speaking, the technique that we introduce is of interest for instance for high-resolution imaging of lithospheric structures at high frequency.
We also introduce and discuss a new exact way of handling viscoelastic dissipation in such full waveform imaging problems [2].

References

[1] Wang, Y., Chevrot, S., Monteiller, V., Komatitsch, D., Mouthereau, F., Manatschal, G., Sylvander, M., Diaz, J., Ruiz, M., Grimaud, F., Benahmed, S., Pauchet, H. and Martin, R., 2016, *The deep roots of the western Pyrenees revealed by full waveform inversion of teleseismic P waves*, Geology, in press.

[2] Komatitsch, D., Xie, Z., Bozdağ, E., Sales de Andrade, E., Peter, D., Liu, Q. and Tromp, J., 2016, *Anelastic sensitivity kernels with parsimonious storage for adjoint tomography and full waveform inversion*, Geophysical Journal International, in press.

HPC Architectures evolution: the case of Marconi, the new Cineca flagship system.

Carlo Cavazzoni
Cineca
via Magnanelli 6/3, 40033 - Casalecchio di Reno Italy
c.cavazzoni@cineca.it

The end of Moore's Law, the little improvement in silicon chips and power constraints are jeopardizing the future of HPC architectures. Moreover, for many datacenters the capacity in term of electrical power is coming to its limit, and without a dramatic improvement in floating point efficiency this limit will determine the maximum size of the high-end system that can be deployed. To plan and sustain the increase of performance of the supercomputers disruptive changes in data centers, architectures and softwares need to be faced. In this talk the architecture design of Marconi, the new flagship system of Cineca will be presented and related to the above challenge. Finally the impact of the new architectures on the applications development for geoscience will be discussed.

HPC strategies for Large Eddy Simulations of volcanic ash plumes

Matteo Cerminara
Istituto Nazionale di Oceanografia e Geofisica Sperimentale
Istituto Nazionale di Geofisica e Vulcanologia
via della Faggiola, 32 56126 - Pisa, Italy
mcerminara@inogs.it

Tomaso Esposti Ongaro
Istituto Nazionale di Geofisica e Vulcanologia
via della Faggiola, 32 56126 - Pisa, Italy
tomaso.espostiongaro@ingv.it

Stella Paronuzzi
Istituto Nazionale di Geofisica e Vulcanologia
via della Faggiola, 32 56126 - Pisa, Italy
stella.paronuzzi@gmail.com

In order to forecast volcanic plumes and ash dispersal in the atmosphere – simulating their turbulent evolution – three-dimensional (3D) computational fluid dynamic models are needed [1, 2]. With this aim, a finite volume solver (ASHEE) for compressible, turbulent dispersed multiphase flows is implemented in the OpenFOAM infrastructure [3, 4].
The evolution of volcanic ash clouds is a multiscale phenomenon, where the largest scales are of the order of tens of kilometers and minutes, while the smallest are microns and microseconds. This wide range of scales makes Direct Numerical Simulations (DNS) of volcanic ash plumes computationally unfeasible. However, Large Eddy Simulations (LES) techniques allow to reduce significantly the number of degrees of freedom to be solved to capture mean and fluctuation properties of such a geophysical-scale flow. This makes modern High Performance Computing (HPC) infrastructures capable to afford in a reasonable time the computational requests of the associated mathematical problem.
The ASHEE model [3] is a compressible formulation of the equilibrium–Eulerian model developed by [5, 6]. It allows to solve efficiently the dynamics of polydisperse mixtures, capturing solid particles clustering phenomena like preferential concentration and turbophoresis. It is faster than standard Eulerian–Eulerian multiphase models [7], but it can be used only for fine enough particles (Stokes number smaller than 0.2).
A variety of subgrid-scale models for LES are implemented in the ASHEE model. They are both static (like the celebrated Smagorinsky-Lilly model) and dynamic (like the Germano dynamic model), offering the possibility to model the subgrid-scale turbulence with and without empirical parameters.
The accuracy of the ASHEE model has been tested against a number of standardized fluid dynamic benchmarks, stressing its capability to capture the physical phenomena involved in the evolution of volcanic ash plumes.
The numerical solver has been used in different HPC infrastructures, up to 1024 cores. This has allowed to model volcanic eruptions with satisfactory resolution within five days

and one month of computational time.
Even if presently its scalability is acceptable, we are working on individuating ASHEE and OpenFOAM bottlenecks, in order to further improve their parallel performances, going towards the possibility to model and forecast volcanic plumes evolution within 24 hours.

References

[1] Costa, A. et al. 2016. *Results of the eruptive column model inter-comparison study.* J. Volcanol. Geotherm. Res., in press.

[2] Suzuki, Y. J. et al. 2016. *Inter-comparison of three-dimensional models of volcanic plumes.* J. Volcanol. Geotherm. Res., accepted.

[3] Cerminara, M., Esposti Ongaro, T. and Berselli, L. C. 2016. *ASHEE-1.0: a compressible, equilibrium–Eulerian model for volcanic ash plumes.* Geosci. Model Dev. 9, 697–730.

[4] Cerminara, M., Esposti Ongaro, T. and Neri, A. 2016. *Large eddy simulation of gas-particle kinematic decoupling and turbulent entrainment in volcanic plumes.* J. Volcanol. Geotherm. Res, accepted.

[5] Maxey, M. R. 1987. *The gravitational settling of aerosol particles in homogeneous turbulence and random flow fields.* J. Fluid Mech. 174, 441.

[6] Ferry, J. & Balachandar, S. 2001. *A fast Eulerian method for disperse two-phase flow.* Int. J. Multiph. flow 27, 1199–1226.

[7] Esposti Ongaro, T. and Cerminara, M. 2016. *Non-equilibrium processes in ash-laden volcanic plumes: new insights from 3D multiphase flow simulations.* J. Volcanol. Geotherm. Res., in press.

Dynamically adaptive tsunami simulations on Xeon Phi architectures

Chaulio Ferreira
Technical University of Munich
Boltzmannstr. 3, 85748 Garching, Germany
chaulio.ferreira@tum.de

Ao Mo-Hellenbrand
Technical University of Munich
Boltzmannstr. 3, 85748 Garching, Germany
hellenbr@in.tum.de

Michael Bader
Technical University of Munich
Boltzmannstr. 3, 85748 Garching, Germany
bader@in.tum.de

$sam(oa)^2$ (Space-filling curves and Adaptive Meshes for Oceanic And Other Applications) is an efficient framework for the solution of 2D partial differential equations using a discretization based on dynamically adaptive triangular grids. It has been implemented using both distributed and shared memory parallelism and has been shown to scale well on up to 8192 cores. One of the application scenarios in $sam(oa)^2$ is based on the Shallow Water Equations and can be used to simulate tsunami wave propagation. In this work, our goal is to improve the performance of this scenario, focusing on Intel® Xeon Phi™ coprocessors. We experiment not only with running $sam(oa)^2$ using a single Xeon Phi™ coprocessor in native mode, but also with executions in symmetric mode, that is, running simulations on nodes with two Xeon Phi™ coprocessors and one Intel® Xeon® Ivy Bridge host processor each.

As a first strategy to improve the simulation efficiency, we implemented the concept of patches: each grid cell is now treated as a triangular "patch" containing regularly refined cells. This strategy improves the simulation performance not only due to more efficient memory accesses, but also allows the implementation of vectorized Riemann solvers, which can take advantage of the new data organization to process all edges in a patch using SIMD instructions. We implemented two versions of such solvers, which achieved up to 2.6× speedup on a single Xeon Phi™ coprocessor, compared to the no-patches version.

Also, using a heterogeneous system may lead to serious load imbalance issues. $sam(oa)^2$ features a load balancing strategy to take care of imbalances due to the dynamic refinement and coarsening during the simulation. However, this strategy distributes the load evenly among all processors, since it considers all processors to have similar efficiency. In order to fully exploit the system's computing power, we are working on improving the load balancing module in $sam(oa)^2$, so that the relative efficiency of each processor is considered explicitly or implicitly. On a single node and using an explicitly fixed load ratio determined empirically, we have been able to reduce the simulation wall time in up to 45%, compared to the naive load balancing that distributes the load evenly. Our current focus is on

implementing a load balancing strategy that can determine the best load ratio for each processor in execution time, thus achieving optimal efficiency in other heterogeneous systems as well. Afterwards, we plan to extend our work to multiple heterogeneous nodes.

Advances in HPC for the NEMO Ocean Model

Silvia Mocavero
Euro-Mediterranean Center on Climate Change Foundation
via Augusto Imperatore, 16 73100- Lecce Italy
silvia.mocavero@cmcc.it

Sandro Fiore
Euro-Mediterranean Center on Climate Change Foundation
via Augusto Imperatore, 16 73100 - Lecce Italy
sandro.fiore@cmcc.it

Giovanni Aloisio
Università del Salento, Dipartimento di Ingegneria dell'innovazione
via per Monteroni, 73100 - Lecce Italy
Euro-Mediterranean Center on Climate Change Foundation
via Augusto Imperatore, 16 73100 - Lecce Italy
giovanni.aloisio@unisalento.it

Access to large computational facilities for ocean modelling is required to meet the need for higher spatial and temporal resolution thus allowing climate change research to improve long-term trends predictions. NEMO [5] is one of the most common ocean models. Unfortunately, to fully exploit the next generation of massive parallel systems, the code should be deeply re-designed exploiting revolutionary co-design approaches. However, some evolutionary techniques can be proposed and adopted to improve the performance of the NEMO legacy code in the short-term, which of course can be highly beneficial for researchers working in production-level environments.
The talk is focused on two main topics: (i) the improvement of the NEMO model parallel efficiency, which means reaching good code scalability on thousands of cores and (ii) the need to increase the single-node peak performance exploitation.
Parallel inefficiency problem is generally addressed through the minimization of the communication overhead and/or the improvement of the workload balance among the parallel processes. Pros and cons of alternative parallel strategies have been investigated in two kernels, respectively resolving the tracer advection and the tracer lateral diffusion [1]; additionally, the best trade-off between communication and computation in one of the most computationally intensive kernel, implementing the SOR (Successive Over Relaxation) algorithm, has been evaluated [2]. Moreover, some optimizations on both the Open Boundaries [3] and the North-Fold algorithm have been designed and implemented, as results of a deep analysis of the main bottlenecks, also performed at routine level. A reduction of the execution time of about 34% in the first case and an improvement of the parallel efficiency of about 30% in the second case, have been achieved.
Finally, the analysis of the code shows that single-node performance are well below the peak performance [4] of modern HPC systems. A deeper investigation at routine level allows identifying memory and computational bounded kernels thus helping the definition of the improvement strategy. It is worth of mentioning that single-node performance could be increased exploiting the memory locality and improving the instruction parallelism.

References

[1] Epicoco, I., Mocavero, S., Porter, A. R., Pickles, S. M., Ashworth, M. and Aloisio, G. 2016 *Hybridisation Strategies and Data Structures for the NEMO Ocean Model*. International Journal of High Performance Computing, to appear.

[2] Epicoco, I., Mocavero, S. and Aloisio, G. 2012 *The performance model for a parallel SOR algorithm using the red-black scheme*. International Journal of High Performance Systems Architecture, vol. 4, p. 101-109, ISSN: 1751-6528.

[3] Epicoco, I., Mocavero, S. and Aloisio, G. 2011 *The NEMO oceanic model: Computational performance analysis and optimization*. In *Proceedings of the 2011 IEEE International Conference on High Performance Computing and Communications*. pp. 382-388, Los Alamitos, CA:IEEE Computer Society, ISBN: 978-076954538-7, doi: 10.1109/HPCC.2011.56

[4] Epicoco, I., Mocavero, S., Macchia, F. and Aloisio, G. 2014 *The Roofline Model for Oceanic Climate Applications*. In *Proceedings of the 2014 IEEE International conference on High Performance Computing & Simulation*. pp. 732-737, ISBN: 978-1-4799-5311-0

[5] Madec, G. and the NEMO team 2008 *NEMO ocean engine.* Note du Pole de modellisation, No. 27, Institut Pierre-Simon Laplace (IPSL), France, ISSN: 1288-1619.

Advances in HPC for Geophysical Applications - Part II

PROPOSERS

Giovanni Tumolo
The Abdus Salam International Centre for Theoretical Physics and OGS
Strada Costiera, 11 34151 - Trieste Italy
gtumolo@ictp.it

Paolo Crosetto
C2SM/CSCS-ETHZ, Zürich
Via Trevano, 100 6900 - Lugano Switzerland
paolo.crosetto@usys.ethz.ch

SPEAKERS

Martin Schreiber
College of Engineering, Mathematics and Physical Sciences, University of Exeter
M.Schreiber@exeter.ac.uk

Florian Prill
Deutsche Wetterdienst, Offenbach, Germany
florian.prill@dwd.de

William Sawyer
CSCS-ETHZ, Lugano , Switzerland
wsawyer@cscs.ch

Paolo Crosetto
C2SM/CSCS-ETHZ, Lugano , Switzerland
paolo.crosetto@usys.ethz.ch

Giovanni Tumolo
The Abdus Salam International Centre for Theoretical Physics and OGS, Trieste, Italy
gtumolo@ictp.it

In order to effectively address the complex multidisciplinary problems arising in geophysics, a wide variety of cross competences is required. Numerical methods are used to solve complex coupled physical models on state of the art supercomputers. In particular the efficient use of supercomputing facilities is of utmost importance for most of the geophysical applications, and the detailed knowledge of the recent trends in supercomputing hardware might affect the choice of the numerical technique employed and of its implementation. For these reasons a close interaction between domain scientists, experts in numerics, and High Performance Computing experts is highly beneficial. With this minisymposium we aim at gathering experts from the three aforementioned fields, namely geophysical science, numerical methods, and HPC, in order to facilitate interactions and to enhance collaborations across the domains.

Dynamic Adaptive Mesh Refinement with RLE-clustering vs. Parallelization-in-Time with REXI

Martin Schreiber
University of Exeter
M.Schreiber@exeter.ac.uk

Solving PDEs is a challenging task and requires redesigning algorithms to reduce the time-to-solution or mathematical formulations to cope with those modern HPC architectures. This talk will discuss two orthogonal methods for solving PDEs and their common optimization target given by the time-to-solution.

The first part of this talk is on using dynamic adaptive mesh refinement (DAMR) with space-filling curves (SFC) [13] which allows using resources more efficiently (time-to-solution, e.g.) by adopting the mesh over runtime to track important features. We developed an efficient *cluster-oriented*[4] parallelization concept. Partitions are described by spatially clustered cells generated by the Sierpinski SFC [12] with partitions being independently stored in the same memory context. We use a run-length encoded buffering strategy for efficient inter-partition communication of edges[9] and nodes[8]. With multiple independent partitions in a single memory, this yields direct support of OpenMP/TBB[9] and the extension to MPI is quasi-optimal via block-wise edge/node data transfer and quasi-optimal RLE-cluster data migration[10]. Additionally, such a parallel software concept allows cluster-based optimizations by dynamic reordering or skipping operations on clusters[11]. Given a *fixed number of computing resources which still allow a scalable parallelization* we will show and discuss results of shallow-water and representative Tsunami simulations with DAMR and the resulting significant reduction in computational workload and time-to-solution.

The second part of this talk will be on one of the parallelization-in-time methods. These methods focus on computations which are already limited in spatial strong-scalability by

[4]The paradigms and algorithms of this parallel software software concept were explained to Prof. Michael Bader in 2011 and led to disruptive changes in the development of the parallelization approach of the so-called $sam(oa)^2$ framework in 2012: The original parallelization approach of the so-called sam(oa)2 development (ver. 2011) only allowed relatively efficient MPI-based edge communication. See e.g. [5] with the MPI parallelization results based on the development of [6] (this was a joint work with Kaveh Rahnema). This parallelization concept of samoa 2 was actively developed until 2012. In contrast, the clustering approach (including plenty of features not possible with the original approach in sam oa 2) was presented and explained to Oliver Meister, Kaveh Rahnema and Prof. Michael Bader in 2011 and further details in 2012 [4]. This concept was named clustering in 2012 since this method would allow efficient cluster-based local time stepping on DAMR triangular grids. After explaining Oliver Meister all the problems of their original approach (e.g. MPI-only, no cluster-based optimizations) and the advantages of the run-length encoding and the parallel software concept, he decided in mid 2012 that "[...] merging the parallelization approach of Kaveh [...] does not make sense. I'm not doing this but I'm now also implementing something which supports cluster-based local time stepping". The interested reader might find updated information regarding the samoa2 development of Prof. Michael Bader, Oliver Meister and Kaveh Rahnema sooner or later here:
http://www.martin-schreiber.info/data/webdata/phd_thesis_html/schreiber14dissertationse20.html#x29-470003

applying strategies which allow to overcome this scalability limitation by using the time as an additional dimension of parallelization. This focuses on reducing the time-to-solution even for applications which are limited by their spatial scalability. We will discuss a parallelization-in-time approach for the oscillatory parts of the shallow water equations which will be parallelized with a massively parallel rational approximation of exponential integrators (REXI)[3]. This yields speedups of two orders of magnitude for problem sizes which would be already *limited in spatial scalability on a single compute node*. A parallel performance model shows scalability on over 100k cores for sufficiently large time step sizes. The source code of both developments is freely available in the repositories [1] and [2].

References

[1] Martin Schreiber et al., https://bitbucket.org/schreiberx/sierpi/

[2] Martin Schreiber et al., https://github.com/schreiberx/sweet

[3] High-order time-parallel approximation of evolution operators, Terry Haut, T. Babb, P. G. Martinsson, B. Wingate

[4] M. Schreiber: What I'm doing or try to do... Sierpi(nski) & more, Chair Meeting 2012, Technical University of Munich, June 2012, `http://www5.in.tum.de/~schreibm/private/thuburn/extracted/dynamic_adaptive_grids/2012_06_13_lst_treffen.pdf`

[5] M. Bader: Parallelization and Software Concepts for Tsunami Simulation on Dynamically Adaptive Triangular Grids, Workshop on Adaptive Multiscale Methods for the Atmosphere and Ocean, Newton Institute for Mathematical Sciences, Cambridge, August 2012, http://www.newton.ac.uk/programmes/AMM/seminars/2012082414301.pdf

[6] Csaba A. Vigh. Parallel Simulation of the Shallow Water Equations on Structured Dynamically. Adaptive Triangular Grids. PhD thesis, Institut fuer Informatik, Technical University of Munich

[7] Behrens, J. and Zimmermann, J., Parallelizing an Unstructured Grid Generator with a Space-Filling Curve Approach, Euro-Par 2000 Parallel Processing, Munich, Germany, Lecture Notes in Computer Science, vol. 1900, Springer Verlag, 2000, pp. 815-823

[8] M. Schreiber, T. Weinzierl und H.-J. Bungartz, SFC-based Communication Metadata Encoding for Adaptive Mesh, Proceedings of the International Conference on Parallel Computing (ParCo), 2013

[9] M. Schreiber, H.-J. Bungartz und M. Bader, Shared Memory Parallelization of Fully-Adaptive Simulations Using a Dynamic Tree-Split and -Join Approach, IEEE Xplore, Puna, India, 2012

[10] M. Schreiber und H.-J. Bungartz, Cluster-based communication and load balancing for simulations on dynamically adaptive grids, In Proceedings of the International Conference on Computational Science (ICCS'14), Elsevier

[11] M. Schreiber, T. Weinzierl und H.-J. Bungartz, Cluster Optimization and Parallelization of Simulations with Dynamically Adaptive Grids, Euro-Par 2013, Lecture Notes in Computer Science, Springer, Berlin, 2013

[12] Bader, M., Schraufstetter, S., Vigh, C.A. and Behrens, J. Memory efficient adaptive mesh generation and implementation of multigrid algorithms using Sierpinski curves

[13] H. Sagan, Space-filling Curves

Quadrature-free Implementation of a Spherical DG Scheme Based on a Local Tangent Basis

Florian Prill
German Weather Service (DWD)
Frankfurter Str. 135, D-63067 Offenbach
florian.prill@dwd.de

Discontinuous Galerkin (DG) methods appear as a suitable candidate for next-generation climate and numerical weather prediction codes. Among the key features of this approach are its high parallel efficiency and geometrical flexibility, justifying the additional complexity of the discretization. However, high-order DG methods have not been used in operational global circulation models yet.
In this context, we present a proof-of-concept study that is aimed at the Icosahedral Nonhydrostatic Model (ICON), the currently operational numerical weather prediction code of the German weather service. Requirements for a DG dynamical core for ICON are discussed in detail.
One important aspect is the careful treatment of the spherical curvature which introduces additional acceleration terms into the discretized fluid conservation laws. While the majority of spherical DG schemes is either based on a spatial transformation of the original equations or the embedding into a global Cartesian coordinate system, we follow Bernard et al. [1] and employ a normalized local tangent basis computed directly from the mapping. This can be interpreted as a DG scheme with non-polynomial shape and test functions. We combine the approach with the quadrature-free CPR scheme [2].
Applied to shallow water flow the resulting test model demonstrates the potential of the DG approach even in this early stage of our dynamical core development.

References

[1] Bernard, P.-E. et al. 2009 *High-order Discontinuous Galerkin Schemes on General 2D Manifolds Applied to the Shallow Water Equations*, J. Comput. Phys., vol. 228, 6514–6535.

[2] Huynh, H. T. 2011 *High-Order Methods Including Discontinuous Galerkin by Reconstructions on Triangular Meshes*, 49th Aerospace Sciences Meeting, AIAA.

What we have learned from porting the ICON General Circulation Model to GPUs

William Sawyer
Swiss National Supercomputing Centre (CSCS)
via Trevano 131, CH-6900 Lugano, Switzerland
wsawyer@cscs.ch

Introduction

CSCS has made a large commitment to port applications from a variety of scientific fields in a way which ensures performance portability across an array of target architectures. In this talk we would like to present the implementation of the Icosahedral Non-Hydrostatic (ICON) model [2], being jointly developed by the Max Planck Institute for Meteorology (MPI-M) and the German Weather Service (DWD), which is becoming increasingly used for simulations in Numerical Weather Prediction (NWP) and Climate Science. We will treat the computational challenges and present the programming techniques — OpenACC/OpenMP directives and MPI message passing — which were ultimately chosen for the high performance implementation.

Climate and Numerical Weather Prediction: the ICON Model

In atmospheric general circulation models (AGCMs), the solution of the equations describing atmospheric *dynamics* — essentially the fully-compressible 3D Euler equations on the sphere — can take the majority of the overall model execution time, depending on the type of algorithm used and the model resolution. The collective effects of physical phenomena which cannot be resolved in the dynamics grid scale are calculated by physical parameterizations (so-called *physics*) on a vertical atmospheric profile of one horizontal grid "box". Together the dynamics and physics form the crux of climate / NWP models. In order to obtain a performant implementation for various HPC architectures, both of these components have to be addressed, usually with differing strategies.
For example, in an AGCM on hybrid-multicore architectures, such as Graphics Processing Units (GPUs), most data must be offloaded from the host to the device outside the main time loop, which contains both dynamics and physics, and updated on the latter until output occurs. Implementing only part of the algorithm on the GPU would necessitate large data transfers of the prognostic and diagnostic fields as they are updated, and this traffic would negate any performance gains from the many cores.
The application under consideration is the Icosahedral Non-hydrostatic (*ICON*) application [2], which is a global and/or regional climate / NWP model currently under development at the German Weather Service (DWD) and the Max Planck Institute for Meteorology (MPI-M). It is being ported to heterogeneous platforms by CSCS using a directive-based approach with both the OpenACC [5] and OpenMP [7] standards for parallelization, and the Message Passing Interface (MPI) for communication.

ICON dynamical core implementations

In a previous paper [1], we presented a comparison of different programming paradigms for ICON on GPUs, namely OpenCL [6], CUDAFortran [3] and OpenACC. It was decided that the latter directive-based approach, which can be incorporated into the existing ICON Fortran code, was the least invasive of the three: Neither OpenCL nor CUDAFortran is transparent to the existing MPI/OpenMP implementation, thus these paradigms would detract from the maintainability. OpenACC admittedly also has its deficiencies, which will be treated subsequently.
We have implemented ICON dynamics with an OpenACC distributed-memory (MPI) implementation alongside the existing OpenMP. We are in the process of augmenting the existing OpenMP physics with OpenACC.

Listing 1: *The gradient calculation in the ICON shared utilities represents a typical triply-nested loop in the dycore. Note that while compilers allow compilation with both OpenMP and OpenACC, parallel regions from the two paradigms cannot overlap. Compilers are capable of inlining the* `get_indices_e` *routine. The calculation is only performed on the MPI processes associated with GPUs (*`i_am_accel_node`*), and only if accelaration has been turned on at runtime (*`acc_on`*). At the end, a call to* `check_patch_array` *illustrates the online validation check with the CPU sequential code (running on a thread with* `.NOT. i_am_accel_node`*), which would not appear in the final code.*

```
#ifdef _OPENACC
!$ACC DATA PCOPYIN( psi_c ), PCOPYOUT( grad_norm_psi_e ), IF( i_am_accel_node .AND. acc_on )
!$ACC PARALLEL, PRESENT( ptr_patch, iidx, iblk, psi_c, grad_norm_psi_e ), IF( i_am_accel_node .AND. acc_on )
!$ACC LOOP GANG
#else
!$OMP PARALLEL
!$OMP DO PRIVATE(jb,i_startidx,i_endidx,je,jk) SCHEDULE(runtime)
#endif
  DO jb = i_startblk, i_endblk
    CALL get_indices_e(ptr_patch, jb, i_startblk, i_endblk, i_startidx, i_endidx, rl_start, rl_end)
!$ACC LOOP VECTOR COLLAPSE(2)
#ifdef __LOOP_EXCHANGE
    DO je = i_startidx, i_endidx
      DO jk = slev, elev
#else
    DO jk = slev, elev
      DO je = i_startidx, i_endidx
#endif
! compute the normal derivative by the finite difference approximation
        grad_norm_psi_e(je,jk,jb) = ( psi_c(iidx(je,jb,2),jk,iblk(je,jb,2)) - &
          &    psi_c(iidx(je,jb,1),jk,iblk(je,jb,1)) ) * ptr_patc
      ENDDO
    ENDDO
  ENDDO
#ifdef _OPENACC
!$ACC END PARALLEL
#ifdef DEBUG_MATH_GRADIENT
!$ACC UPDATE HOST( ptr_delp_mc_new ), IF( i_am_accel_node )
    CALL check_patch_array(SYNC_E,p_patch, grad_norm_psi_e), ``grad_norm_psi_e'')
#endif
!$ACC END DATA
#else
!$OMP END DO NOWAIT
!$OMP END PARALLEL
#endif
```

The step into mainstream code development revealed numerous weaknesses in OpenACC, which would tend to bring its efficacy as a viable heterogeneous multicore programming paradigm into question. Listing 1 reveals that instances of derived types are used in the innermost loops which need to be vectorized on the GPU. This implies that these instances need to be deep-copied to the GPU at the beginning of the time integration loop.

Support for full deep copy of derived types was not available in OpenACC 2.0 [4], and, despite extensive lobbying, was not included in OpenACC 2.5 [5], though it is envisaged for OpenACC 3.0. We have relied on a preliminary and unsupported implementation of full deep copy, part of the Cray CCE 8.3.x compiler.
Next, OpenACC compilers do not currently support class member functions which are allowed in the Fortran 2003 standard. This is crucial in some physical parameterizations currently being ported.

Listing 2: *ICON makes frequent use of index lists of grid points with fulfill a particular condition. The sequential construction of the list prohibits its vectorization, but fortunately in the ICON dycore, all instances of the criterion test and the application of grid point lists could be replaced with an immediate application within the test. Unfortunately the following list from the advection algorithm needs to be applied to numerous tracers and thus cannot be avoided. Thus the counter is protected with an* `ACC ATOMIC` *clause, with performance implications.*

```
ie = 0
!$ACC LOOP VECTOR COLLAPSE(2)
DO jk = slev, elev
  DO je = i_startidx, i_endidx
    ! logical switch for MERGE operations: .TRUE. for p_vn >= 0
    lvn_pos     = p_vn(je,jk,jb) >= 0._wp
    ! compute length of backward trajectory
    traj_length = SQRT(p_vn(je,jk,jb)**2 + p_vt(je,jk,jb)**2) * p_dt
    ! distance from edge midpoint to upwind cell circumcenter [m]
    e2c_length  = MERGE(ptr_
      &                 ptr_
    IF (traj_length > 1.25_wp*e2c_length) THEN   ! add point to index list
!$ACC ATOMIC UPDATE
      ie = ie + 1
!$ACC END ATOMIC
      opt_falis
      opt_falis
    ENDIF
  ENDDO ! loop over edges
ENDDO   ! loop over vertical levels
! store list dimension
opt_falis
```

Finally, the code makes repeated use of *grid-point lists* (listing 2), namely lists of indices for which a given grid-point condition is fulfilled. These grid lists were successfully replaced in the dycore, but they are not easily removable from the other sections of ICON, for example the advection algorithm in question. In this case, the `!$ACC ATOMIC` directive can be used effectively, with little performance impact.
The success of OpenACC is completely dependent on the expression of sufficient multi-level parallelism in the code. As Listing 1 reveals, ICON developers had the foresight to implement a blocking factor `nproma` (`je` loop, $1 \leq$ `i_startidx` $\leq$ `i_endidx` $\leq$ `nproma`) and array indexing (local index, level, block id) which performs adequately on both CPU and GPU, albeit with different values of `nproma` (CPU optimum 8 – 32, GPU optimum 128 – 1024, depending on resolution). Moreover, most intern loop pairs (`je, jk`) can be exchanged by setting a compiler flag. With the appropriate compilation and proper `nproma` values, the single-socket Intel Sandybridge + NVIDIA K20x nodes outperform dual-socket Intel Haswell nodes (Figure 1) by a factor commensurate to the ratio of obtainable memory bandwidth, typical for such bandwidth-limited calculations.

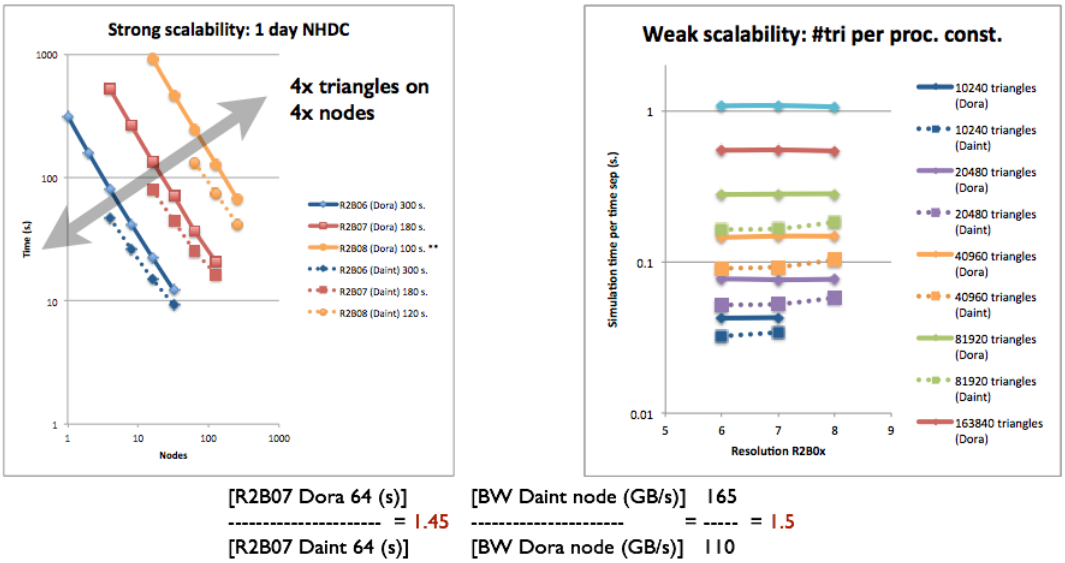


Figure 1: *The strong (left) and weak (right) scalability of the ICON dycore is compared for dual-socket Haswell nodes (solid lines) vs. hybrid Sandybridge/K20x nodes (dashed lines) for three different global resolutions. GPU strong scalability is worse than for CPU, but when the global grid just fits into GPU memory, e.g., 64 nodes for R2B05, the timings ratio is comparable to the ratio of achievable bandwidths from the stream benchmark (bottom).*

Summary

In this abstract we have illustrated some of the implementation issues in the combined OpenACC/OpenMP+MPI implementation of the ICON dynamics, which allow it to run efficiently on CPU and GPU architectures. We look forward to presenting this work at the SIMAI conference, as well as the ongoing project to port the ICON physics with the same paradigm.

References

[1] W. Sawyer, A. Kozhevnikov, and R. Solcà, *Utilizing Hybrid Programming Environments: CSCS Case Studies*. In **Parallel Computing: On the Road to Exascale**. ISBN 978-1-61499-620-0, 663–672 (2016).

[2] G. Zängl, D. Reinert, P. Ripodas, and M. Baldauf, *The ICON (ICOsahedral Non-hydrostatic) modelling framework of DWD and MPI-M: Description of the non-hydrostatic dynamical core*. QJRMS **141** (687), 563–579 (2015).

[3] *CUDA Fortran Programming Guide and Reference*. `https://www.pgroup.com/doc/pgicudaforug.pdf`. 2015.

[4] *The OpenACC Application Programming Interface, Version 2.0 (corrected)*. `http://www.openacc.org/sites/default/files/OpenACC.2.0a_1.pdf`. August, 2013.

[5] *The OpenACC Application Programming Interface, Version 2.5 (public comment version)*.

`http://www.openacc.org/sites/default/files/OpenACC_2dot5_draft_for_public_comment_0.pdf`. August, 2015.

[6] J. E. Stone, D. Ghoara, and G. Shi, *OpenCL: A Parallel Programming Standard for Heterogeneous Computing Systems*. IEEE Des. Test **12** (3), 66–73 (2010).

[7] L. Dagum and R. Menon. OpenMP: An Industry-Standard API for Shared-Memory Programming. *IEEE Transactions on Computational Science and Engineering*, 5(1), 1998.

Performance Portable Numerics using GridTools

Paolo Crosetto
ETH Zürich
via Trevano, 131 - Lugano Switzerland
paolo.crosetto@usys.ethz.ch

Mauro Bianco
CSCS
via Trevano, 131 - Lugano Switzerland
m.bianco@cscs.ch

Carlos Osuna
MeteoSwiss
Zürich airport - Zürich Switzerland
carlos.osuna@meteoswiss.ch

GridTools is a collection of C++ libraries for the development of grid applications, like PDE solvers on block-structured grids. The main driving applications for GridTools are complex real-world problems arising in geophysical science, which need to be efficiently parallelized on modern architectures, such as accelerators. GridToools is the successor of STELLA [3] a library used to discretize and accelerate the dynamical core of the COSMO weather model. GridTools's goal is to provide more general purpose tools, allowing the user to define different types of grids, implement different discretization schemes (e.g. Galerkin discretizations), while exposing a more abstract API which can easily adapt to different application domains.
The GridTools libraries are written in C++, which allows, via generic programming and template metaprogramming techniques, to abstract many of the core concepts which depend on the underlying architecture, like preferred memory layout, memory hierarchy, and preferred parallel programming models. Currently NVIDIA GPU and X86 backends are supported. A python JIT compiler is implemented together with the core C++ library as an environment for rapid prototyping. The modular software architecture of the libraries is shown in figure 1. The project is founded by the PASC[5] intiative. Below are some of the optimization strategies implemented in the GridTools core library:

- X86 (OpenMP):
  - Loop tiling: consists in partitioning the iteration space into tiles fitting in the cache memory, and loop over one tile at a time. This technique enhances data locality and improves caches utilization.
  - Loop fusion: This technique consists in performing multiple loops over one tile at a time.This leads to better performance, but it requires the tiles to be overlapping, the overlap being a halo region set up by the library based on a data dependency analysis. When temporary storages are needed in order to store intermediate results, these can be instantiated with the size of a tile,

[5]Platform for Advanced Scientific Computing http://www.pasc-ch.org/

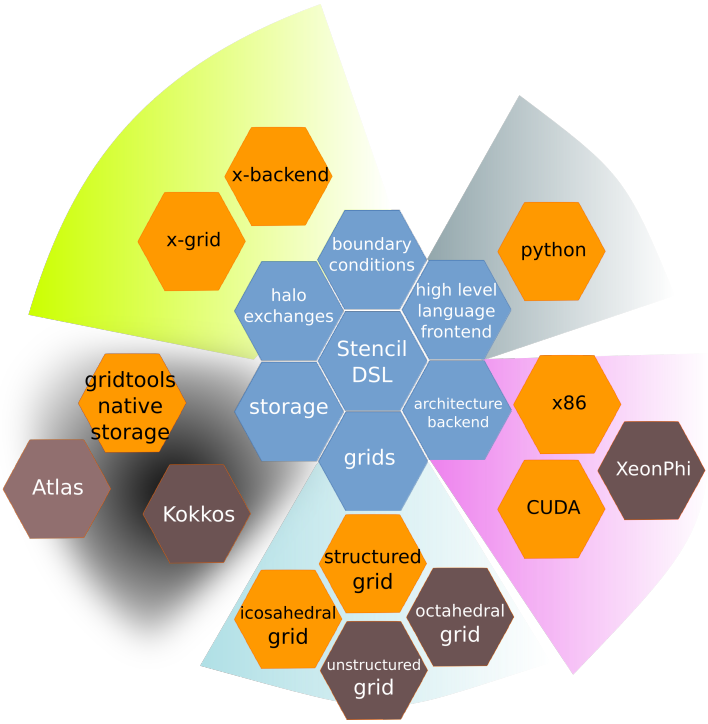


Figure 1: The central part in blue shows the core components of GridTools, the generic layer which is common to all the tools. The orange components represent implementations of more specific features. The brown exagones show possible external contributions, third party libraries, or future extentions.

therefore fitting in the CPU cache. This algorithm allows a better utilization of the CPU caches, see [1] for details.

- Alignment: the API exposes an interface to properly set the data alignment, in order to exploit vectorization on the architectures supporting it.

- GPU (CUDA)
  - Stage fusion: consists in having the possibility of merging multiple computation stages which are logically separated into a single execution kernel. This kernel performs all the stages either sequentially or concurrently, depending on the data dependency.
  - Data locality: the GPUs do not have traditional coherent caches for access to non constant data, for this purpose the GPU shared memory is used to read-write data which is frequently accessed (e.g. the loop logic resources, the value of temporary fields).
  - Read only data cache: loading data through the texture unit allows us to take advantage of the GPU's read only data cache.
  - Optimization of resources of the loop logic: the size of the objects accessed in the innermost loop is crucial on a GPU, due to the limited amount of available resources per thread. In order to reduce the register pressure GridTools implements mechanisms to keep such memory consumption low.

– Alignment: On the GPU unaligned access to the data still produces an overhead. GridTools makes sure that all accesses to global memory are properly aligned.

1 The API

The GridTools API consists in two main parts: the definition of the user function, executed at each iteration point (possibly on the device), see Figure 2, and the definition of the computation, see Figure 4. The instantiation and definition of the storages is also required, and shown in Figure 3. Additional available features of the core library include

```
struct flux_x {
    using tmpx=accessor<0,inout,extent<>, 4>;
    using sol=accessor<1,in,extent<0,-1>, 4>;
    using arg_list=boost::mpl::vector<tmpx,sol> ;
    using comp=dimension<4>;

    template <typename Evaluation>
    static void Do(Evaluation const & eval, z_interval) {
        double dx=0.01, dt=0.02, g=9.81;
        dimension<1>::Index i;
        using hx=alias<tmpx,comp>::set<0>; using h=alias<sol,comp>::set<0>;
        using ux=alias<tmpx,comp>::set<1>; using u=alias<sol,comp>::set<1>;
        using vx=alias<tmpx,comp>::set<2>; using v=alias<sol,comp>::set<2>;
        eval(hx{})= eval((h{}+h{i-1})/2. -
                         (u{}-u{i-1})*(dt/(2*dx)));
        eval(ux{})=eval((u{} + u{i-1})/2.-
                        ((pow<2>(u{})/h{}+pow<2>(h{})*g/2.)-
                         (pow<2>(u{i-1})/h{i-1} +
                          pow<2>(h{i-1})*(g/2.)
                             ))*(dt/(2.*dx)));
        eval(vx{})=eval((v{} + v{i-1})/2. -
                        (u{}*v{}/h{} - u{i-1}*v{i-1}/h{i-1})*(dt/(2*dx)) );
    }
};
```

Figure 2: GridTools implementation of the firt step of the shallow waters problem in [2]. The accessors are placeholders for the storages, and they are defined given a policy (input or output), an extent (specifying the access pattern), and a dimension (4 in this case). The extents are used in a data dependency analysis step performed at compile time, which computes the amount of *halo* points needed. The `alias` keyword statically assigns a name to an accessor at a specific dimension offset.

conditional switches (i.e. stages are enabled or disabled based on the value of a run-time condition), reduction operations, stencil functions (possibility to nest user funcitions), boundary conditions assignment, generic accessors (accessing a user-defined object from the user function), support for non-cartesian grids (e.g. icosahedral grid on the sphere), and several others. Among the extentions being developed as a usage example of the GridTools API we mention a toolchain for high order Finite Elements assembly and Krylov solvers. The MPI-CUDA, or MPI-OpenMP programming models are supported via the Generic Communication Layer (GCL), which is also part of the GridTools.

```
using info_t=backend<Cuda,Block>::storage_info<0,layout_map<2,1,0>>::type;
using sol_t=backend<Cuda,Block>::storage_type<float,info_t>::type;
using tmp_t=backend<Cuda,Block>::temporary_storage_type<float,info_t>::type
    ;
info_t info_(d1, d2, d3);
using sol_vec_t = field<sol_t, 1, 1, 1>::type;
using tmp_vec_t = field<tmp_t, 1, 1, 1>::type;
sol_vec_t sol_(info_, 0., "solution [h,u,v]")
using p_sol=arg<0,sol_vec_t>;
using p_tmpx=arg<1,tmp_vec_t>;
using p_tmpy=arg<2,tmp_vec_t>;
using arg_list = boost::mpl::vector<p_sol, p_tmpx, p_tmpy>;
aggregator_type<arg_list> aggregator_((p_sol() = sol_));
```

Figure 3: This snippet shows how to initialize the storages in case of the *shallow water* operator described in [2]. The specific backend and algorithm is selected using the `Cuda` and `Block` keywords. The `storage_info` object contains the dimensions and strides for the storages (in this case all storages have the same structure). The type `sol_vec_t` represents a list of storages of size 3 ((h, u, v) in [2]), while `p_sol` is a placeholder for this storage list. The placeholders `p_tmpx` and `p_tmpy` are temporary (i.e. the associated storage contains intermediate results). They are managed automatically by the library.

```
auto shallow_water = make_computation<gridtools::BACKEND>
    (   aggregator_, grid_,
        make_stencil
        (   execute<forward>(),
            define_caches(cache<IJ, p_tmpx, p_tmpy, local>()),
            make_independent(make_stage<flux_x>(p_tmpx(), p_sol() ),
                             make_stage<flux_y>(p_tmpy(), p_sol() )),
            make_stage<final_step>(p_tmpx(), p_tmpy(), p_sol() )
    ));
    shallow_water.ready(); //allocates temporaries (if any)
    shallow_water.steady(); //copy data to device if needed
    shallow_water.run(); //executes
    shallow_water.finalize(); //copy results back, cleanup
```

Figure 4: This snippet represents the definition of the tree of execution for the *shallow water* operator described in [2]. Notice that the the temporary storages are cached between two consecutive stages.

References

[1] Bianco, M. and Cumming, B. 2014 A generic strategy for multi-stage stencils. In *Euro-Par 2014 Parallel Processing* pp. 584–595. Springer International Publishing.

[2] Moler, C. 2011 Experiments with MATLAB. *http://ch.mathworks.com/moler/exm/chapters/water.pdf* chap. 18. pub-MATHWORKS.

[3] Gysi, T. and Osuna, C. and Fuhrer, O. and Bianco, M. and Schulthess, T. C. 2015 STELLA: A Domain-specific Tool for Structured Grid Methods in Weather and Climate Models. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis (SC'15)* pp. 41:1–41:12. ACM

A strategy for parallelization of high order p-adaptive DG methods

Giovanni Tumolo
The Abdus Salam International Centre for Theoretical Physics and OGS
Strada Costiera, 11 34151 - Trieste Italy
gtumolo@ictp.it

Luca Bonaventura
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
luca.bonaventura@polimi.it

Graziano Giuliani
The Abdus Salam International Centre for Theoretical Physics
Strada Costiera, 11 34151 - Trieste Italy
ggiulian@ictp.it

One of the main issues encountered in parallelization of dynamic p-adaptive high order local Galerkin discretizations of time dependent problems is represented by the load unbalance which may be generated at runtime. We will present a strategy aimed at designing a flexible parallelization for dynamic p-adaptive dicontinuous Galerkin formulations, which makes easier the migration of elements between processes in order to keep the load distribution across processors as much balanced as possible when the number of degrees of freedom employed in each element is adapted at runtime. Preliminary results will be shown in order to assess the effectiveness of the proposed approach. Future developments and applications to geophysical fluid dynamics modeling problems will be also discussed.

Mathematical and numerical modeling of heart functioning and systemic circulation - Part I

PROPOSERS

Luca Dedé
Chair of Modelling and Scientific Computing, MATHICSE, École Polytechnique Fédérale de Lausanne
Av.Piccard, Station 8, CH-1015 Lausanne, Switzerland
luca.dede@epfl.ch

Andrea Manzoni
Chair of Modelling and Scientific Computing, MATHICSE, École Polytechnique Fédérale de Lausanne
Av.Piccard, Station 8, CH-1015 Lausanne, Switzerland
andrea.manzoni@epfl.ch

Simone Scacchi
Dipartimento di Matematica, Università di Milano
Via Saldini, 50, 20133 Milano, Italy
simone.scacchi@unimi.it

Christian Vergara
MOX, Dipartimento di Matematica, Politecnico di Milano
Piazza Leonardo da Vinci 32, 20133 - Milano Italy
christian.vergarai@polimi.it

SPEAKERS

Lucia Gastaldi
Dipartimento di Ingegneria Civile, Architettura,Territorio, Ambiente e di Matematica, Università degli Studi di Brescia, Italy
lucia.gastaldi@unibs.it

Salvatore Pasta
Fondazione Ri.MED, Palermo, Italy
spasta@fondazionerimed.com

Christian Contarino
Department of Civil, Environmental and Mechanical Engineering, University of Trento, Italy
christian.contarino@unitn.it

Elena Faggiano
Department of Civil Engineering and Architecture, University of Pavia, Italy
elena.faggiano@gmail.com

Simone Morganti
Dipartimento di Ingegneria Industriale e dell'Informazione, University of Pavia, Italy
simone.morganti@unipv.it

Davide Forti
Chair of Modelling and Scientific Computing, MATHICSE, École Polytechnique Fédérale de Lausanne, Switzerland
davide.forti@epfl.ch

Cardiac and Cardiovascular Mathematics represents nowadays a challenging topic in view of the emerging and growing collaborations between clinicians and mathematicians. In this respect, the numerical solution of problems arising in modeling cardiac and systemic phenomena opens new and interesting perspectives which need to be properly addressed. From the cardiac side, a fully integrated heart model represents a complex multiphysics problem, which is in turn composed of several submodels describing cardiac electrophysiology, mechanics, and fluid dynamics. Each submodel exhibits a spatial and temporal multiscale behavior and poses significant mathematical, numerical and computational challenges. While the systemic circulation has been studied for a longer time, several mathematical and numerical aspects still need to be addressed, as e.g. tissue remodeling, atherosclerotic plaque formation, aneurysms development, transitional and turbulence phenomena in blood flows. This minisymposium aims at gathering researchers and experts in mathematical and numerical modeling of the heart and the systemic circulation at large. Topics include, but are not limited to cardiac models, including electrophysiology, mechanical activation, fluid dynamics of the heart, valve modeling, patient-specific and image-based simulations, as well as fluid-structure interaction in real and large vessels, turbulence models, tissue growth and remodeling.

A fictitious domain approach with a Lagrange multiplier for fluid-structure interactions

Lucia Gastaldi
Università degli Studi di Brescia
Piazza del Mercato, 15 25121 - Brescia Italy
lucia.gastaldi@unibs.it

Daniele Boffi
Università degli Studi di Pavia
Strada Nuova, 65 27100 - Pavia Italy
daniele.boffi@unipv.it

Numerical schemes for fluid-structure interaction problems include interface fitted meshes (thus requiring suitable remeshing in order to keep the fluid computational grid aligned with the interface) or interface non-fitted meshes (allowing to keep the fluid computational grid fixed and independent from the position of the solid). The immersed boundary method (see [5] for a review) is a typical example of non-fitted schemes. It has been introduced in the 70's for the simulation of biological problems related to the blood flow in the heart and it has been extended to finite elements in a series of papers starting from [2] by using a variational approach FE-IBM. In particular, in [4] the original fiber-like description of the structure has been abandoned in favor of a more natural and intrinsically *thick* modeling of the solid domain. With this representation, a unified treatment of immersed structures is possible in any combination of dimensions. In [1] a new formulation DLM-IBM for fluid-structure interaction problems has been introduced based on the FE-IBM which makes use of a distributed Lagrange multiplier in the spirit of the fictitious domain method. An important feature of the DLM-IBM, is that its semi-implicit time discretization results to be unconditionally stable as opposed to the standard FE-IBM where a suitable CFL condition has to be satisfied. The time discretization of the problem leads to a saddle point problem and we consider its finite element discretization. We present a rigorous analysis showing that both continuous and discrete saddle point problems are stable and that the discrete solution converges optimally towards the continuous one (see [3] for more details).

References

[1] D. Boffi, N. Cavallini, and L. Gastaldi. The finite element immersed boundary method with distributed Lagrange multiplier. *SIAM J. Numer. Anal.*, 53(6):2584–2604, 2015.

[2] D. Boffi and L. Gastaldi. A finite element approach for the immersed boundary method. *Comput. & Structures*, 81(8-11):491–501, 2003. In honour of Klaus-Jürgen Bathe.

[3] D. Boffi and L. Gastaldi. A fictitious domain approach with distributed Lagrange multiplier for fluid-structure interactions. *Numer. Math.*, 201

[4] D. Boffi, L. Gastaldi, L. Heltai, and C. S. Peskin. On the hyper-elastic formulation of the immersed boundary method. *Comput. Methods Appl. Mech. Engrg.*, 197(25-28):2210–2231, 2008.

[5] C. S. Peskin. The immersed boundary method. *Acta Numer.*, 11:479–517, 2002.

Modelling Right Heart Failure in Patients with Pulmonary Hypertension

Salvatore Pasta
Fondazione RIMED
Via Bandiera,11 - 90133 Palermo, Italy
sap62@pitt.edu

Francesco Scardulla
DICGIM, Università degli studi di Palermo
Viale delle Scienze, 8, 90128 Palermo Italy
francesco.scardulla@unipa.it

Piero Mercadante
DICGIM, Università degli studi di Palermo
Viale delle Scienze, 8, 90128 Palermo Italy

Diego Bellavia
IRCCS ISMETT
Via Tricomi n.5, 90128, Palermo, Italy
dbellavia@ismett.edu

Cesare Scardulla
IRCCS ISMETT
Via Tricomi n.5, 90128, Palermo, Italy
cscardulla@ismett.edu

Pulmonary hypertension (PH) is a pathological condition in which the mean pulmonary artery pressure is higher than the normal condition. This condition may ultimately lead to right ventricle failure (RVF). Standard of care in precapillary pulmonary hypertension includes serial right ventricular catheterizations in order to monitor RV performance and pulmonary bed pressures, unfortunately with associated costs and side effects related to invasive procedures [1]. Our aim was two-fold: 1) to develop a biventricular finite-element model coupled to a lumped-parameter circulatory system of PH; 2) to assess accuracy of proposed computational model in predicting hemodynamic impairment due to PH and abnormal motion of interventricular septum [2, 3, 4]. Results showed a good agreement between lumped- and catheter-related hemodynamic measures and the ability of our biventricular model to capture the systolic abnormal motion of interventricular septum observed clinically. This may allow less invasive clinical procedure and rapid computational prediction for the diagnosis of PH. Further studies on large patient cohort are warranted to refine model and confirm results.

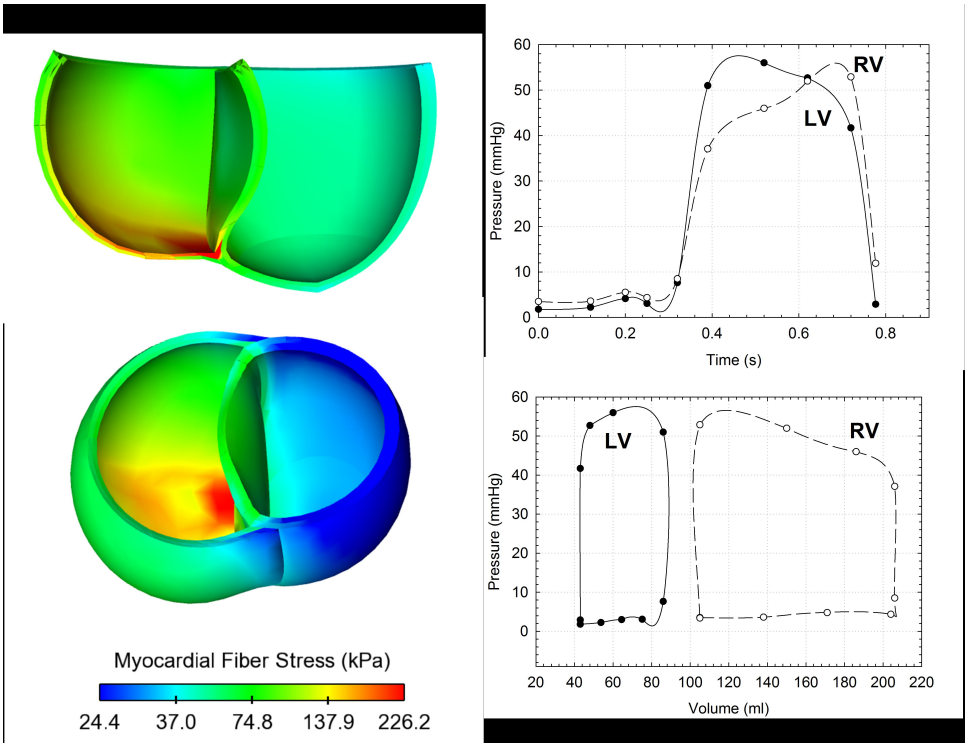


Figure 1: End-systolic myocardial wall stress showing abnormal motion of interventricular septum (left); pressure-time and pressure-volume loop obtained by the lumped-parameter model (right).

References

[1] Bourji, K.I. and P.M. Hassoun, 2015 *Right ventricle dysfunction in pulmonary hypertension: mechanisms and modes of detection.* Curr Opin Pulm Med. **21** (5): p. 446-53.

[2] Lumens, J. and T. Delhaas 2012 *Cardiovascular modeling in pulmonary arterial hypertension: focus on mechanisms and treatment of right heart failure using the CircAdapt model.* Curr Am J Cardiol. **110** (6 Suppl): p. 39S-48S..

[3] Scardulla, F., et al. 2016 *Evaluation of ventricular wall stress and cardiac function in patients with dilated cardiomyopathy.* Proc Inst Mech Eng H, **230** (8): p. 807-18.

[4] Wenk, J.F., et al. 2013 *A coupled biventricular finite element and lumped-parameter circulatory system model of heart failure.* Comput Methods Biomech Biomed Engin, **16** (8): p. 807-18.

A one-dimensional mathematical model for dynamically contracting collecting lymphatics: first steps towards a model for the human lymphatic network

Christian Contarino
Università degli Studi di Trento
via Sommarive, 14 38123 - Povo (Trento) Italy
christian.contarino@unitn.it

Eleuterio F. Toro
Università degli Studi di Trento
eleuterio.toro@unitn.it

In recent years, mathematical models for the circulatory systems have been made huge steps forward and this is particularly true for the arterial system [4]. Very recently, such models have taken a further step, to incorporate more fluid compartments, e.g. microvasculature, venous system and the cerebrospinal fluid, see [8, 9, 10, 1]. In all of these developments, the lymphatic system has been largely neglected, though recent works [7, 5, 2, 6] have started to make significant progress in this area. However, there is a huge gap between these initial works and the ambitious aim of constructing a global mathematical model for the full lymphatics network coupled to all relevant fluid compartments.
Here we design a new one-dimensional mathematical model for collecting lymphatics coupled with an enhanced FitzHugh-Nagumo model for the contractibility of the lymphatic wall [3]. The contraction model does not depend on a prescribed contractile function, but is rather based on a set of Ordinary Differential Equations (ODEs) which describe the action potential and the state for contraction for each lymphangion. The model is based on three mechanisms: (1) environmental calcium influx, (2) stretch activated calcium influx and (3) contraction inhibitions induced by wall shear stresses. Numerical results show that the model is able to reproduce the trend of available experimental measurements. The mathematical model reproduces the rhythmic, spontaneous lymphatic contraction that generates the pressure needed to open the downstream valve, see Figs. 1 and 2. We simulated different combinations of upstream and downstream pressures, and the resulting frequencies are reported in Fig. 3. Results for a human-like lymphatic network will be shown, see Fig. 4.

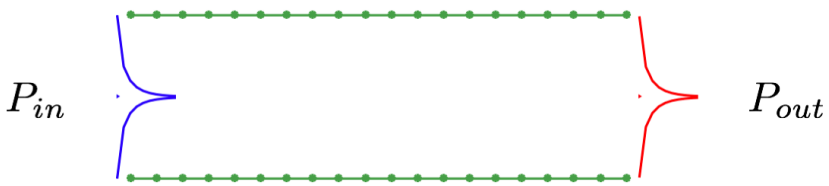


Figure 1: Illustration of a sectioned lymphangion: a single contractile lymphatic vessel bounded by two valves at the extremities.

References

[1] P. J. Blanco, S. M. Watanabe, E. A. Dari, M. A. R. F. Passos, and R. A. Feij´oo. Blood flow distribution in an anatomically detailed arterial network model: criteria and algorithms. Biomechanics and Modeling in Mechanobiology, 13(6):1303–1330, 2014.

[2] A. W. Caulk, J. B. Dixon, and R. L. Gleason. A lumped parameter model of mechanically mediated acute and long-term adaptations of contractility and geometry in lymphatics for characterization of lymphedema. Biomechanics and Modeling in Mechanobiology, apr 2016.

[3] C. Contarino and E. F. Toro. A one-dimensional mathematical model for dynamically contracting collecting lymphatics. Manuscript in preparation

[4] L. Formaggia, A. Quarteroni, and A. Veneziani. Cardiovascular Mathematics. Modeling and simulation of the circulatory system. Springer, 2009.

[5] S. Jamalian, M. J. Davis, D. C. Zawieja, and J. E. Moore. Network scale modeling of lymph transport and its effective pumping parameters. PLOS ONE, 11(2):e0148384, feb 2016.

[6] C. Kunert, J. W. Baish, S. Liao, T. P. Padera, and L. L. Munn. Mechanobiological oscillators control lymph flow. Proceedings of the National Academy of Sciences, 112(35):10938–10943, aug 2015.

[7] A. J. MacDonald, K. P. Arkill, G. R. Tabor, N. G. McHale, and C. P. Winlove. Modeling flow in collecting lymphatic vessels: one-dimensional flow through a series of contractile elements. American Journal of Physiology-Heart and Circulatory Physiology, 295(1):H305–H313, 2008.

[8] L. O. Mueller and E. F. Toro. A global multiscale mathematical model for the human circulation with emphasis on the venous system. International Journal for Numerical Methods in Biomedical Engineering, 30(7):681–725, 2014.

[9] L. O. Mueller and E. F. Toro. Enhanced global mathematical model for studying cerebral venous blood flow. Journal of Biomechanics, 47(13):3361–3372, 2014.

[10] J. P. Mynard and J. J. Smolich. One-dimensional haemodynamic modeling and wave dynamics in the entire adult circulation. Annals of Biomedical Engineering, 43(6):1443–1460, apr 2015.

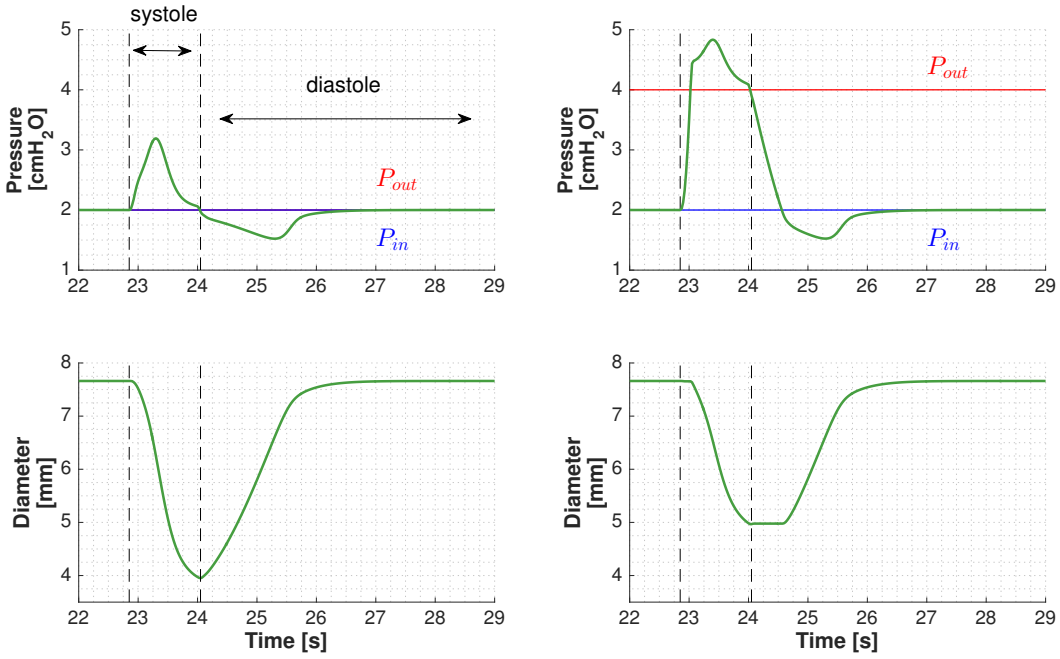


Figure 2: Time-varying mean pressure and mean diameter of a single lymphangion. Two different cases for the upstream and downstream pressure were simulated. The left column depicts the numerical result using equal pressures ($P_{in} = P_{out} = 2$ cmH$_2$O). The right column depicts the numerical result with the downstream pressure greater than the upstream one ($P_{in} = 2$ cmH$_2$O and $P_{out} = 4$ cmH$_2$O).

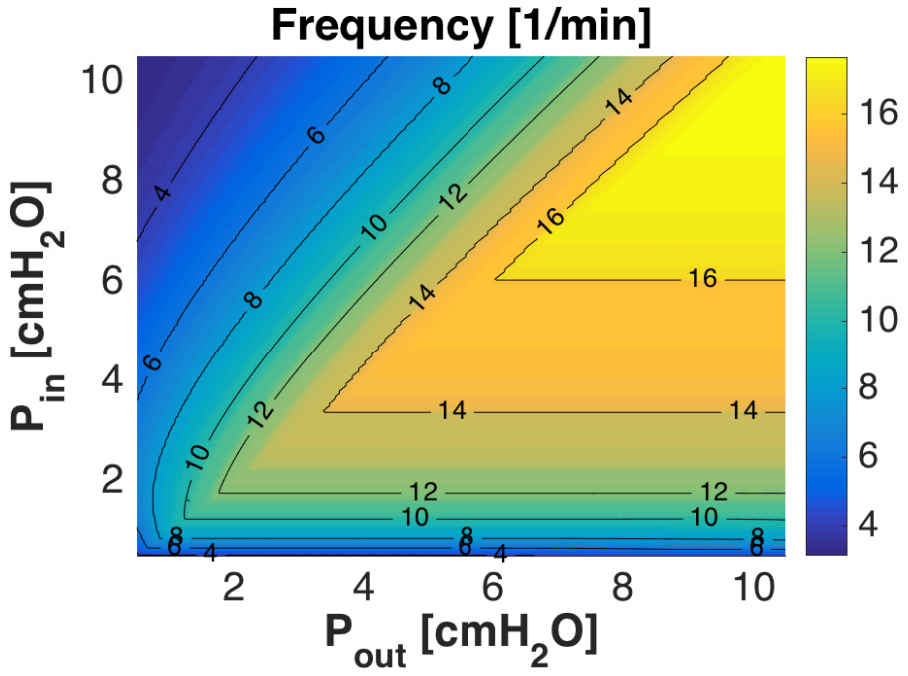


Figure 3: Frequencies resulting from different combinations of upstream and downstream pressures in a single lymphangion.

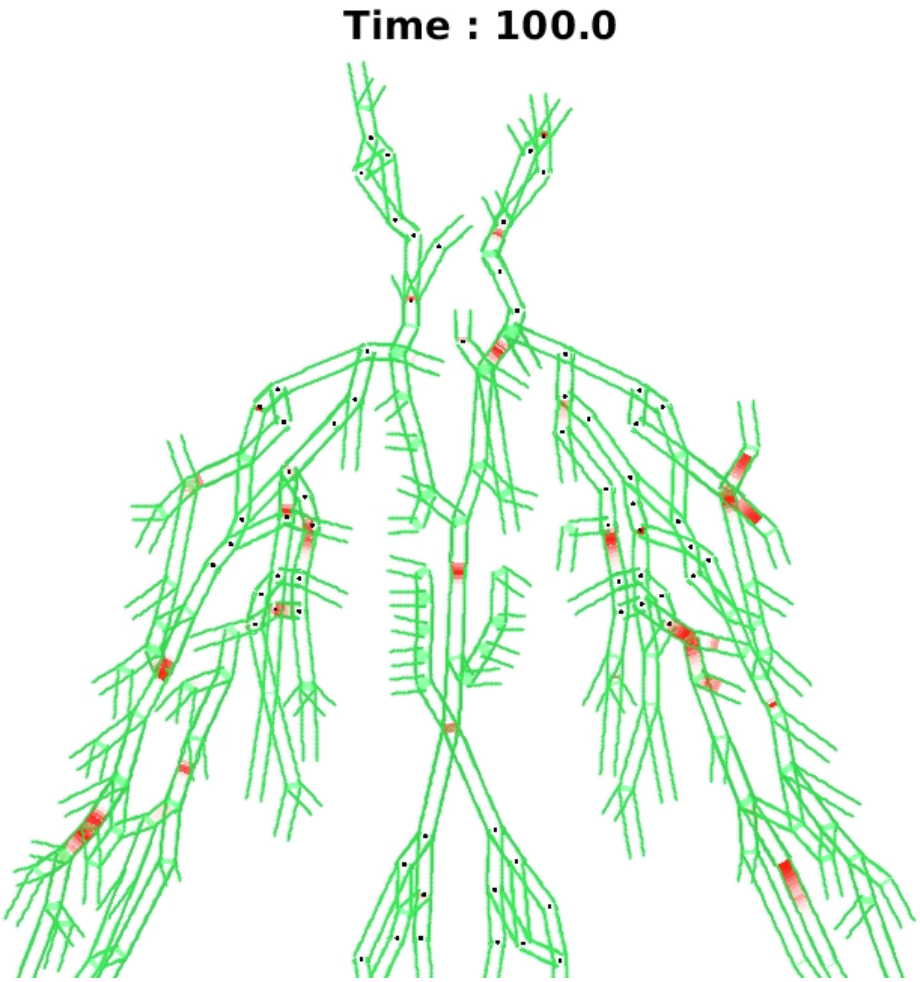


Figure 4: Example of a human-like lymphatic network. Red color depicts contracted lymphangions.

A study of the Cardiatis Multilayer Flow Modulator: from in-vivo geometrical analysis to patient-specific simulations

Elena Faggiano
University of Pavia
Via Ferrata, 3 27100 - Pavia Italy
elena.faggiano@unipv.it

Alice Finotello
University of Genova,
Via Leon Battista Alberti, 2 16132 Genova Italy

Marco Fedele
University of Pavia
Via Ferrata, 3 27100 - Pavia Italy

Gianluca Alaimo
University of Pavia
Via Ferrata, 3 27100 - Pavia Italy

Michele Conti
University of Pavia
Via Ferrata, 3 27100 - Pavia Italy

Simone Morganti
University of Pavia
Via Ferrata, 3 27100 - Pavia Italy

Ferdinando Auricchio
University of Pavia
Via Ferrata, 3 27100 - Pavia Italy

Open surgery of thoraco-abdominal aortic aneurysm (TAAA) is the gold standard approach for treating such pathology but, endovascular aortic implantation can be considered a valuable alternative for patients who are not eligible for such an invasive procedure. The Cardiatis Multilayer Flow Modulator (MFM) is an uncovered, self-expanding stent made of braided cobalt-alloy wire (Phynox) used to treat aortic aneurysms. Its main feature is to change the blood flow within the aneurysm, modifying turbulent to laminar flow, reducing the wall shear stress and maintaining perfused the side branches. Its aim consists also in supporting the formation of organized, stable thrombus inside the aneurysm sac, contributing to stop the growth of the aneurysm and to decrease the risk of aneurysm rupture.
In the medical literature, controversial studies analyzing the follow-up of groups of patients treated with the MFM are available [2], while engineering studies of the same subject are

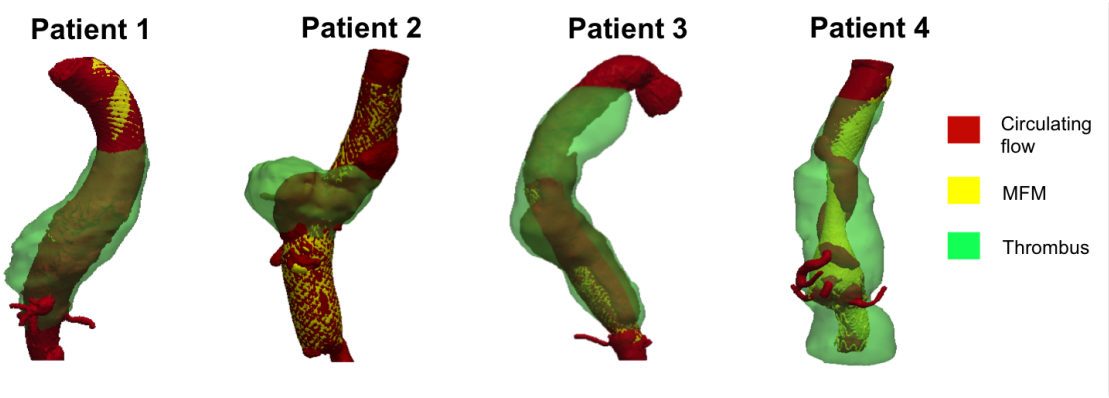


Figure 1: 3D reconstructions of the images of four patients acquired directly after the implantation of the MFM stent.

not in literature. In this context, a full engineering framework for the analysis of the MFM device represents an innovation. The study is intended to help clinicians understanding the feasibility of the intervention in TAAA using this novel device and interpreting the post-operative (short and long term) outcomes.
The study aims to develop two different frameworks: (i) a tool to perform advanced in-vivo geometrical analysis to support the clinicians in the evaluation of the aneurysm evolution; (ii) a patient-specific simulation framework which considers the porosity of the MFM in order to investigate the hemodynamics changes after the implantation.
Concerning the in-vivo geometrical analysis, we reconstruct the circulating flow, the MFM and the thrombus geometries from medical images (see Figure 1) and we analyze their changes in time introducing new descriptive and synthetic indices such as section areas (lumen and aneurysm), total aneurysm volume, aneurysm growth rate, residual flow volume, total flow growth rate, and thrombization rate index. Concerning the simulation framework, we model the MFM as a porous surface and we perform numerical simulations using the Resistive Immersed Implicit Surface model [1]. More in particular, to describe the MFM porosity, we perform an in-vitro study in a 3D printed y-model inserting one or two MFM inside it; then, we tune the resistance of the numerical model performing numerical simulations in the same y-model (see Figure 2).

References

[1] Fedele, M. and Faggiano, E. and Dedé, L. and Quarteroni, A. 2016 *A patient-specific aortic valve model based on moving resistive immersed implicit surfaces.* Biomech. Model. in Mechanobiol., submitted.

[2] Henry, M. and Benjelloun, A. and Henry, I. 2015 *The multilayer flow modulator stent for the treatment of arterial aneurysms.* Handbook of Interventions for Structural Heart and Peripheral Vascular Disease, pp. 317.

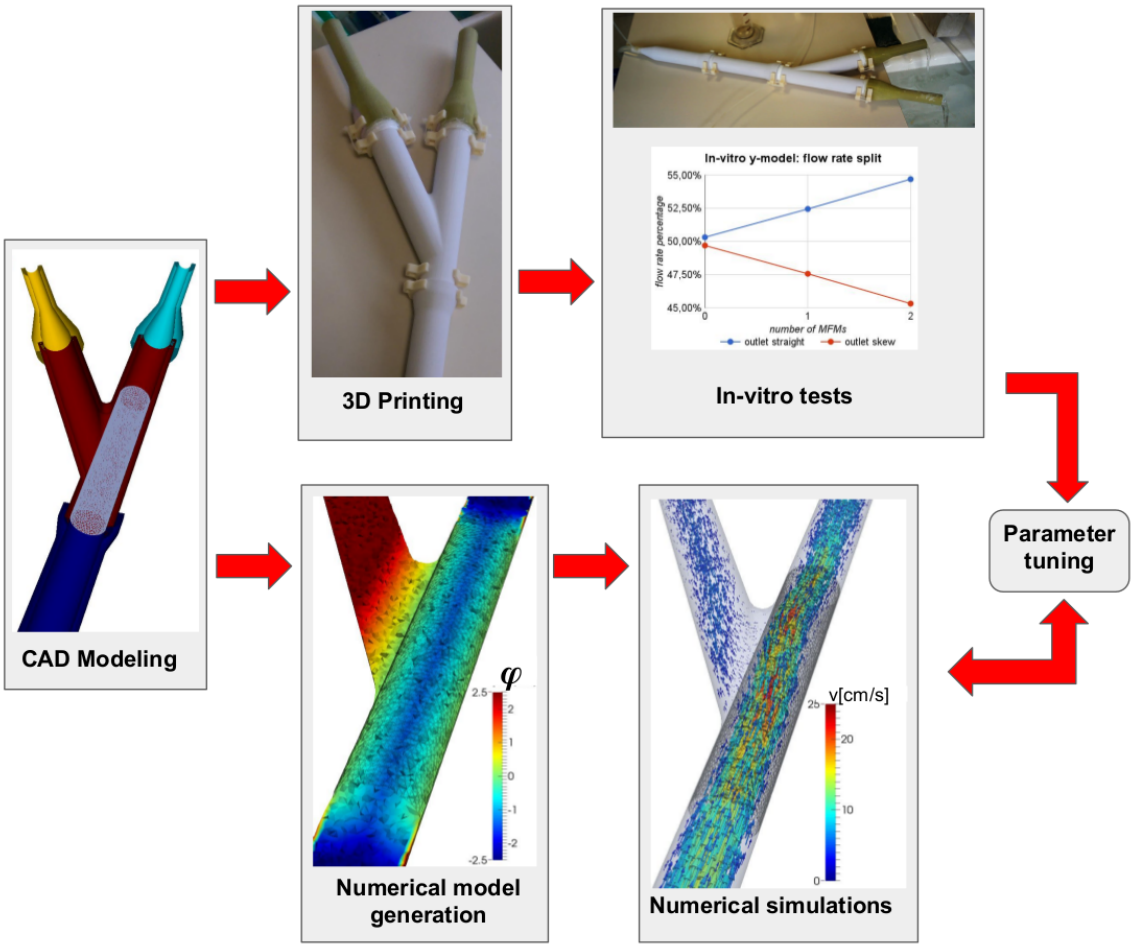


Figure 2: A sketch of the simulation framework.

Predictive simulation framework for thoracic aortic endograft implantation: virtual deployment and CFD analysis

Simone Morganti
Università degli Studi di Pavia
via Ferrata, 5 27100 - Pavia Italy
simone.morganti@unipv.it

Michele Conti
Università degli Studi di Pavia
via Ferrata, 3 27100 - Pavia Italy
michele.conti@unipv.it

Elena Faggiano
Università degli Studi di Pavia
via Ferrata, 3 27100 - Pavia Italy
elena.faggiano@unipv.it

Rodrigo Romarowski
Università degli Studi di Pavia
via Ferrata, 3 27100 - Pavia Italy
rodrigo.romarowski@unipv.it

Ferdinando Auricchio
Università degli Studi di Pavia
via Ferrata, 3 27100 - Pavia Italy
auricchio@unipv.it

Thoracic endovascular aortic repair (TEVAR) is nowadays a consolidated alternative to open surgery to treat aortic diseases such as aneurysms and dissections [1]. A correct pre-operative planning is essential for positive long-term outcomes of the procedure and to avoid drawbacks such as endoleaks. Diseased thoracic aorta is characterized by complex and tortuous geometries with high inter-individual variability; even the selection of simple geometrical variables of the endograft such as length and diameter could be cumbersome. Motivated by such considerations, in this work we propose a framework to simulate the stent deployment within an aorta creating then the computational mesh to perform fluid-dynamics simulations. The final result is a well fitted geometry representing the fluid dynamics scenario as it would be after the surgery. We conclude that the proposed framework, sketched in Figure 1, is a key step to simulate TEVAR in order to predict stent malappositions and to evaluate post-surgery complications.

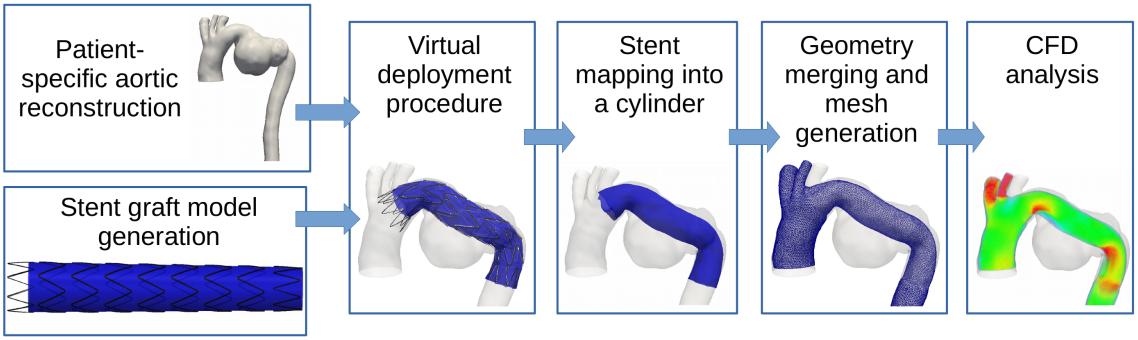


Figure 1: From medical images to analysis: Flowchart summary followed to perform computational analyses of patient-specific TEVAR

References

[1] Auricchio F, Conti M, Marconi S, Reali A, Tolenaar JL, Trimarchi S 2013 *Patient-specific aortic endografting simulation: from diagnosis to prediction.* Comput Biol Med 43(4):386–394

Parallel preconditioners for fluid-structure interaction problems arising in cardiac applications

Davide Forti
EPFL - MATHICSE - CMCS
Av. Piccard, Station 8, CH1015 - Lausanne Switzerland
davide.forti@epfl.ch

Luca Dedè
EPFL - MATHICSE - CMCS
Av. Piccard, Station 8, CH1015 - Lausanne Switzerland
luca.dede@epfl.ch

Simone Deparis
EPFL - MATHICSE
Av. Piccard, Station 8, CH1015 - Lausanne Switzerland
simone.deparis@epfl.ch

Antonello Gerbi
EPFL - MATHICSE - CMCS
Av. Piccard, Station 8, CH1015 - Lausanne Switzerland
antonello.gerbi@epfl.ch

Alfio Quarteroni
EPFL - MATHICSE - CMCS
Av. Piccard, Station 8, CH1015 - Lausanne Switzerland
alfio.quarteroni@epfl.ch

In this talk we present a new block parallel preconditioner for coupled Fluid-Structure Interaction (FSI) problems arising in cardiac applications. The preconditioner is called FaCSI to indicate that it exploits the factorized form of the linearized FSI matrix after spatial and time discretization, as well as the use of static condensation and the SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) preconditioner for saddle-point problems. FaCSI is built upon a block Gauss-Seidel factorization of the exact FSI Jacobian matrix and it uses ad-hoc preconditioners based on domain decomposition or the multigrid method for each physical component of the fully coupled problem. After assessing the parallel performance of FaCSI on benchmark problems, we apply it in the context of large-scale simulations of FSI problems involving the cardiac muscle and the blood flow in the left ventricle of the human heart.

Mathematical and numerical modeling of heart functioning and systemic circulation - Part II

PROPOSERS

Luca Dedé
Chair of Modelling and Scientific Computing, MATHICSE, École Polytechnique Fédérale de Lausanne
Av.Piccard, Station 8, CH-1015 Lausanne, Switzerland
luca.dede@epfl.ch

Andrea Manzoni
Chair of Modelling and Scientific Computing, MATHICSE, École Polytechnique Fédérale de Lausanne
Av.Piccard, Station 8, CH-1015 Lausanne, Switzerland
andrea.manzoni@epfl.ch

Simone Scacchi
Dipartimento di Matematica, Università di Milano
Via Saldini, 50, 20133 Milano, Italy
simone.scacchi@unimi.it

Christian Vergara
MOX, Dipartimento di Matematica, Politecnico di Milano
Piazza Leonardo da Vinci 32, 20133 - Milano Italy
christian.vergarai@polimi.it

SPEAKERS

Matteo Ioriatti
Dipartimento di Ingegneria Civile Ambientale e Meccanica, University of Trento, Italy
matteo.ioriatti@unitn.it

Paola Causin
Dipartimento di Matematica, Università di Milano, Italy
paola.causin@unimi.it

Nicola Cavallini
MathLab, Sissa, Trieste, Italy
nicola.alessandro.cavallini@sissa.it

Fabrizio Del Bianco
Dipartimento di Ingegneria Industriale e dell'Informazione, University of Pavia, Italy
fabrizio.delbianco01@universitadipavia.it

Antonello Gerbi
Chair of Modelling and Scientific Computing, MATHICSE, École Polytechnique Fédérale de Lausanne, Switzerland
antonello.gerbi@epfl.ch

Bruno Guerciotti
MOX, Dipartimento di Matematica, Politecnico di Milano, Italy
bruno.guerciotti@polimi.it

Cardiac and Cardiovascular Mathematics represents nowadays a challenging topic in view of the emerging and growing collaborations between clinicians and mathematicians. In this respect, the numerical solution of problems arising in modeling cardiac and systemic phenomena opens new and interesting perspectives which need to be properly addressed. From the cardiac side, a fully integrated heart model represents a complex multiphysics problem, which is in turn composed of several submodels describing cardiac electrophysiology, mechanics, and fluid dynamics. Each submodel exhibits a spatial and temporal multiscale behavior and poses significant mathematical, numerical and computational challenges. While the systemic circulation has been studied for a longer time, several mathematical and numerical aspects still need to be addressed, as e.g. tissue remodeling, atherosclerotic plaque formation, aneurysms development, transitional and turbulence phenomena in blood flows. This minisymposium aims at gathering researchers and experts in mathematical and numerical modeling of the heart and the systemic circulation at large. Topics include, but are not limited to cardiac models, including electrophysiology, mechanical activation, fluid dynamics of the heart, valve modeling, patient-specific and image-based simulations, as well as fluid-structure interaction in real and large vessels, turbulence models, tissue growth and remodeling.

High Order Semi-implicit Staggered DG schemes for pipe flow simulations

Matteo Ioriatti
Università degli Studi di Trento
via Mesiano 77, 380123 Trento Italy
matteo.ioriatti@unitn.it

Michael Dumbser
Università degli Studi di Trento
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
michael.dumbser@unitn.it

In this framework, the semi-implicit staggered Discontinuous Galerkin (DG) approach proposed by Dumbser and Casulli in [1] is applied in order to discretize two systems of partial differential equations for barotropic fluids in compliant pipes. These methods works very well also in the incompressible limit and consequently it is very sweetable for blood flow simulations
At first, the DG scheme is applied to the one dimensional model for hydrostatic flows which is composed by the continuity and momentum equations in longitudinal direction. The model is closed by two equations of state, one for density and one for the moving wall. Moreover, in order fit experimental results, the unsteady component of the wall shear stress plays a significant role.
Later on, the same numerical approach is applied to a differential model for a two-dimensional hydrostatic and axially symmetric flow. In this case friction models aren't necessary and, consequently, the numerical solution of this model gives a very high resolution structure of the radial velocity profile.
In both cases the pressure is given by solving a mildly non-linear and symmetric system which is efficiently Newton algorithm of Brugnano and Casulli (see [2]).
The two schemes are Arbitrary High order of accuracy in space, while second order of accuracy in time in reached by using the well known theta-method. Moreover, the schemes are unconditionally stable when the convective terms are neglected, otherwise the CFL stability condition of the schemes is based on the fluid velocity. In addition, the schemes behaves very well in the limit of incompressible fluid in rigid tube ($Ma = 0$), where most of classical explicit methods doesn't work. Furthermore, when piecewise constant test functions (N=0) the first order semi-implicit finite volume scheme exposed in [3] is obtained.
The schemes are applied in order to reproduce steady and unsteady analytical solutions in rigid and elastic pipes.

References

[1] M. Dumbser, V. Casulli *A staggered semi-implicit spectral discontinuous Galerkin scheme for the shallow water equations.* Applied Mathematics and Computations vol 219, 8057-8077, 2013.

[2] L. Brugnano, V. Casulli *Iterative solution of piecewise linear systems and applications to flows in porous media.* SIAM Journal on Scientific Computing, vol 31, 1858-1873 , 2009.

[3] M. Dumbser, U. Iben, M. Ioriatti *An efficient semi-implicit finite volume method for axially symmetric compressible flows in compliant tube.* Applied Numerical Mathematics, vol 89, 24-44, 2015.

Mathematical and computational modeling of local blood perfusion: the role of microcirculatory districts

Paola Causin
Dipartimento di Matematica, Università degli Studi di Milano
via C. Saldini, 50 20133 - Milano Italy
paola.causin@unimi.it

Francesca Malgaroli
Dipartimento di Matematica, Politecnico di Milano
piazza Leonardo da Vinci, 32 20133 - Milano Italy
francesca.malgaroli@polimi.it

Introduction

The ability of single body's organs to bring about large selective variations in the rate of blood perfusion relies on the sophisticated regulatory mechanisms of the peripheral circulatory districts. These districts -organized into arterioles, capillaries, and venules- include thousands of vessels with diameter inferior to 200 microns. Blood flow regulation is obtained by variation of the vessel diameter, under the action of both passive and active regulatory mechanisms. We focus our discussion on the first set of mechanisms, investigating the role of geometrical and structural (the so-called "physical") factors in flow regulation. The key point in this process is compliancy: elastic microvessels subjected to mechanical loads deform the structure of their wall, altering the shape of the domain offered to blood and, ultimately, resistance to flow.

Mathematical models of hemodynamics in compliant vessels are present in literature since the 1960s. Nowadays, they are well assessed tools in the simulation of flow in single vessels of major size like the aorta and collaterals, possibly coupled with reduced–order models for the rest of the district of interest. However, in the context of microcirculation, the importance of keeping into account in detail the whole network, made of an exceedingly large number of vessels, makes the problem pretty different. Typically, models of microcirculation may use, on the one side, lumped compartmental descriptions with simplified phenomenological models (see, *e.g.*, [5, 1]) or, on the other, they may concentrate on small networks with sophisticated models, possibly posed in the 3D space and anatomically accurate (see, *e.g.*, [3]). What is lost in the first case is the spatial distribution of field variables, and in the second the complexity of the interactions in the complete large network, both important features of in microcirculation networks. In this contribution, stemming from our recent work on the eye retinal circulation [2], we propose a multiscale mathematical model of large microcirculatory beds described as graph networks of distensible tubes. In each tube, we model blood flow by a generalized Ohm's law, featuring a conductivity parameter function of the area and of the shape of the tube cross section. The vessel deformed geometry is computed according to a structural model for the vessel wall, which includes the possibility of bifurcating behaviors, like

buckling of the vessel under compressive loads in the section. The resulting problem is a nonlinear system of equations, with conductivity representing the fluid–structure cross talk element.

Geometry model

The geometry of a microcirculatory network can be extracted from digitized images in living beings, for example computed tomography angiography scans, or can be constructed *ex–novo* on a computer. For the modeling viewpoint adopted in this work, once the 1D skeleton of the network is obtained and topological connectivity structures are available, there is no difference in the treatment of a geometry, irrespectively from its original source. The simulation tests presented in this works are carried out on computer-generated networks, consisting in asymmetrically branching networks. To fix ideas, we focus on the microcirculatory district of the eye retina. The geometrical properties are chosen so that the network fluid-dynamical field correctly reproduces *in vivo* experimental data in humans. Vessels are generated according to fractal laws, with branching defined by the Murray's law with exponent m. Following [4], we assume that a father vessel with diameter D_f bifurcates into two daughter vessels with diameters D_{d_1} and D_{d_2} given by

$$D_{d_1} = c_{d_1/f} D_f, \qquad D_{d_2} = D_f (1 - c_{d_1/f}^m)^{1/m}, \tag{1}$$

where $c_{d_1/f}$ is an asymmetry coefficient. To improve the accuracy of the computation, additional nodal points may be added in each vessel, delimiting a series of segments.

Blood flow model

Each vessel segment is modeled as a distensible straight duct with (fixed) length L, cross section A and wall thickness h. The cross section has arbitrary shape and is kept constant along the segment axial length. We establish in the vessel segment a system of cylindrical coordinates (r, θ, z). Blood circulation is represented as the steady flow of an incompressible viscous fluid with dynamic viscosity μ. We let p be the luminal fluid pressure, u the axial (and only) velocity component. According to the Poiseuille flow model, mass conservation and momentum balances read

$$\frac{du}{dz} = 0, \qquad -\frac{\partial p}{\partial z} + \mu \triangle_{r\theta} u = 0, \qquad \text{in} \quad \Omega_f = A \times L, \tag{2}$$

$\triangle_{r\theta}(\cdot)$ being the Laplacian restricted to the (r, θ) variables. No–slip boundary conditions hold on $\partial A \times L$. Introducing the dimensionless variables $r^* = r/\widehat{R}$ and $u^* = -\mu u/(\widehat{R}^2 \dfrac{\partial p}{\partial z})$, $\widehat{R}$ being a characteristic length of the cross section, the second equation in (2) reduces in the domain $A^* = A/(\pi \widehat{R}^2)$ to the 2D problem

$$\triangle_{r^*\theta} u^* = -1, \tag{3}$$

along with the no–slip boundary condition on ∂A^*. We let now $Q = \displaystyle\int_A u \, dA$ be the volumetric flow rate. Recalling the above normalizations, the flow can be also written as

$$Q = -\frac{dp}{dz} \frac{\widehat{R}^4}{\mu} \int_{A^*} u^* dA^*, \tag{4}$$

u^* being the solution of problem (3). Relation (4) has the form of a generalized Ohm's law of the type $Q = -\sigma \dfrac{dp}{dz}$, with conductivity σ (inverse of resistance per unit length) defined by

$$\sigma = \frac{\widehat{R}^4}{\mu} \int_{A^*} u^* dA^*. \tag{5}$$

The conductivity is, thus, a characteristic parameter of the tube which depends on the geometry of the (arbitrary) cross section. This latter, in turn, is determined in our framework by the pressure loads acting on the luminal and external sides of the vessel wall, respectively.

Structure model

We model vessel segments as elastic rings made of incompressible material and in the regime of small deformations. Arterioles are generally subjected to positive transmural pressure (difference between luminal and external pressure) and they maintain a circular shape. The deformed radius is thus computable in closed form from mechanical equilibrium and a straightforward use of relation (5) provides the value of the conductivity of the deformed section. Different is the situation for the venules. If, on the one hand, the small wall thickness to radius ratio of venules allows to use a simplified model, which reduces the structure thickness to its midline, on the other, a bifurcation exists in the mechanical behavior. As a matter of fact, a critical value of the transmural pressure exists, which represents the so-called point of buckling. Namely, we distinguish between: *i)* pre-buckling conditions, where the tube cross section deforms under the pressure load but maintains its natural circular shape. Mechanical equilibrium of stresses in the hoop direction yields the well known Laplace's law and, again, the conductivity can be computed analytically from (5); *ii)* buckling point, where the cross section loses its circular shape due to a physical instability phenomenon and buckles with a snap-like action into a non–circular shape; *iii)* post-buckling conditions, where the cross section progressively deforms and significantly reduces the enclosed area for flow. In this conditions, bending of the section must also be kept into account, referring to the elastica equations. A numerical solution is then sought and once the geometry of the deformed cross section is available, we solve (3) by a finite element approximation. The conductivity is then obtained from (5) via numerical quadrature.

Solution procedure

Once the model has been established on a single vessel, coupling conditions must be enforced to obtain network coherence. Namely, pressure continuity and flux conservation must hold at junctions. The following nonlinear boundary value system of PDEs is then to be solved in the union of the fluid domains Ω_f: given the connectivity of the network, the external pressure, the unloaded configuration and the mechanical properties of the vessels, find the flow Q satisfying the network coupling conditions and the continuous pressure p such that in each segment it holds

$$\frac{dQ}{dz} = 0, \qquad Q = -\sigma(p)\frac{dp}{dz}. \tag{6}$$

It is convenient to think that the discrete counterpart of (6) corresponds to the adoption of a primal mixed finite element, in which fluxes are represented as linear functions and

pressures as piecewise linear functions globally continuous, thus ensuring the automatic satisfaction of the pressure coupling condition in the network. The numerical solution of the fully coupled problem on the network is then carried out with a fixed point procedure to solve for nonlinearities.

Simulations results

We study the influence of the asymmetry of the network by considering four different networks with progressively increasing symmetry (that is, with increasing index $c_{d_1/f}$), till reaching a symmetric dichotomic network $c_{d_1/f} = 0.784$. We set the inlet pressure of the network to 40 mmHg, the outlet pressure to 18 mmHg and the external pressure to 20 mmHg. In Tab. 1, we report in the first three rows the the values of the fixed geometrical characteristics of the networks (total number of vessels, min and max route distance of the leaves of the tree). Then, in the last two rows, we report the total cross section and equivalent resistance of the network as obtained from our model after deformation. The observed trends show as more asymmetric networks, asymmetry being a commonly found feature of microcirculatory vessels, offer least resistance than more regular, symmetric structures. This element has a strong important when considered in relation to the several pathologies which severely disrupt the functional organization of microcirculation.

	Asymmetry index $c_{d_1/f}$				trend
Parameter	0.5	0.6	0.7	0.784	
total number of vessels	15252	12415	9664	8191	↘
min route distance [μm]	$1.65 \cdot 10^3$	$1.84 \cdot 10^3$	$2.36 \cdot 10^3$	$3.13 \cdot 10^3$	↗
max route distance [μm]	$1.23 \cdot 10^4$	$7.17 \cdot 10^3$	$4.49 \cdot 10^3$	$3.13 \cdot 10^3$	↘
total cross section [μm^2]	$9.65 \cdot 10^5$	$7.33 \cdot 10^5$	$5.85 \cdot 10^5$	$5.17 \cdot 10^5$	↘
eq. resistance [cm^3/s/mmHg]	$7.84 \cdot 10^{-7}$	$1.14 \cdot 10^{-6}$	$1.43 \cdot 10^{-6}$	$1.7 \cdot 10^{-6}$	↗

Table 1: Characteristic values of parameters of networks (arterial side only) generated by different degrees of asymmetry in branching (increasing symmetry moving to the right, 0.784=symmetry). The last column indicates the trend of each parameter for increasing symmetry. Parameters undergo variations determined by increasing homogeneity of the network, relation between radius and vessel length, constraint of not threspassing the minimal diameter of 5 μm. These elements combined together result into an equivalent resistance which is more than doubled passing from $c_{d_1/f} = 0.5$ to $c_{d_1/f} = 0.784$.

References

[1] Carlson, B., Arciero, J., Secomb, T. (2008). *Theoretical model of blood flow autoregulation: roles of myogenic, shear-dependent, and metabolic responses.* Am. J. Physiol.: Heart Circ. Physiol. 295(4), pp.H1572-9

[2] Causin, P., Guidoboni, G., Malgaroli, F., Sacco, R., Harris, A. (2016). *Blood flow mechanics and oxygen transport and delivery in the retinal microcirculation: multiscale mathematical modeling and numerical simulation.* Biomech. Model. Mechanobiol., 15(3), pp.525-42

[3] Heil, M., Hazel, A. (2015). *Flow in Flexible/Collapsible Tubes.* In "Fluid-Structure Interactions in Low-Reynolds-Number Flows", Chapter 8, C. Duprat and H. Stone Eds., Royal Society of Chemistry

[4] Takahashi, T. (2014) *Microcirculation in fractal branching networks.* Springer Japan

[5] Ursino, Mauro and Lodi, Carlo Alberto (1997). *A simple mathematical model of the interaction between intracranial pressure and cerebral hemodynamics.* J. Appl. Physiol. 82(4), 1256–1269

Distributed Lagrangian Multiplier Formulation of the Finite Element Immersed Boundary Method

Nicola Cavallini
SISSA
via Bonomea, 265 34136 - Trieste Italy
nicola.cavallini@sissa.it

The Immersed Boundary Method (IBM) is a mechanical formulation of fluid-structure interaction problems. It has been introduced in the seventies by C. S. Peskin (see [7] and the references therein). IBM method is methodologically dual to the ALE method. In the second case the fluid is surrounded by the structure. As the structure deforms the fluid domain deforms accordingly. In case of large topological changes the ALE method fails since the remeshing of the deformed domain is not computationally cost effective. With the IBM method the structure is "immersed" in fluid domain. As a consequence fluid and the structure domain discretizations are completely decoupled . Several formulations has been introduced in recent years. In this work we focus on the finite element formulation of this problem [2, 5, 3, 1, 6].
In the finite elements framework we introduced the a Lagrange multiplier for the kinematic condition [4], the condition ensuring the matching of the fluid and the structure velocities. This methodological evolution comes with several benefits on the stability and diffusivity of the method. Preliminary results will be presented on preconditioning the resulting saddle point problem.

References

[1] D. Boffi, N. Cavallini, and L. Gastaldi. Finite element approach to immersed boundary method with different fluid and solid densities. *Math. Models Methods Appl. Sci.*, 21(12):2523–2550, 2011.

[2] D. Boffi and L. Gastaldi. A finite element approach for the immersed boundary method. *Comput. & Structures*, 81(8-11):491–501, 2003. In honour of Klaus-Jürgen Bathe.

[3] D. Boffi, L. Gastaldi, L. Heltai, and C. S. Peskin. On the hyper-elastic formulation of the immersed boundary method. *Comput. Methods Appl. Mech. Engrg.*, 197(25-28):2210–2231, 2008.

[4] Daniele Boffi, Nicola Cavallini, and Lucia Gastaldi. The finite element immersed boundary method with distributed lagrange multiplier. *SIAM Journal on Numerical Analysis*, 53(6):2584–2604, 2015.

[5] L. Heltai. On the stability of the finite element immersed boundary method. *Comput. & Structures*, 86(7-8):598–617, 2008.

[6] L. Heltai and F. Costanzo. Variational implementation of immersed finite element methods. *Comput. Methods Appl. Mech. Engrg.*, 229/232:110–127, 2012.

[7] C. S. Peskin. The immersed boundary method. *Acta Numer.*, 11:479–517, 2002.

Insights on the electromechanical effects of cardiac hypertrophy

Fabrizio Del Bianco
Department of Electrical, Computer and Biomedical Engineering, University of Pavia
via Ferrata, 1 27100 - Pavia Italy
fabrizio.delbianco01@universitadipavia.it

Piero Colli Franzone
Department of Mathematics, University of Pavia
via Ferrata, 1 27100 - Pavia Italy
piero.collifranzone@unipv.it

Simone Scacchi
Department of Mathematics, University of Milano
via Saldini, 50 20133 - Milano Italy
simone.scacchi@unimi.it

Lorenzo Fassina
Department of Electrical, Computer and Biomedical Engineering, University of Pavia
via Ferrata, 1 27100 - Pavia Italy
lorenzo.fassina@unipv.it

Cardiac hypertrophy may be a pathological remodeling caused by a long-term pressure or volume overload inside ventricles [3]. The main phenotypic consequence is a progressive intracellular deposition of new sarcomere units in parallel or in series to the preexistent ones (as modeled, for instance, in [2]). In the present work, we study how this growth correlates with changes in the electromechanical response of the cardiac tissue. Our strongly-coupled electromechanical model joins together an electrophysiological model, an active tension generation model and a finite elasticity model. The electrical activity depends on the mechanical deformation through mechanoelectric feedbacks, see [1]. The space discretization of our model is achieved by trilinear finite elements, whereas the time discretization by a decoupled semi-implicit method. Simulations are run on the Linux cluster of the Department of Mathematics of the University of Milan (https://cluster.mat.unimi.it/). The electromechanical code is written in FORTRAN 90 and parallelized by means of PETSc libraries from the Argonne National Laboratory (http://www.mcs.anl.gov/petsc).

References

[1] Colli Franzone, P. Pavarino, L. F. and Scacchi, S. 2016 *Bioelectrical effects of mechanical feedbacks in a strongly coupled cardiac electro-mechanical model.* Math. Mod. Meth. Appl. S. 26, 27–57.

[2] Göktepe, S. Abilez, O. J. Parker, K. K. and Kuhl, E. 2010 *A multiscale model for eccentric and concentric cardiac growth through sarcomerogenesis.* J. Theor. Biol. 265, 433–442.

[3] Taber, L. A. 1995 *Biomechanics of growth, remodeling, and morphogenesis.* Appl. Mech. Rev. 48, 487–545.

Mathematical and Numerical Models for Integrated Heart Simulations

Antonello Gerbi
CMCS-MATHICSE-SB, École Polytechnique Fédérale de Lausanne
Station 8, CH-1015 Lausanne, Switzerland
antonello.gerbi@epfl.ch

Davide Forti
CMCS-MATHICSE-SB, École Polytechnique Fédérale de Lausanne
Station 8, CH-1015 Lausanne, Switzerland
davide.forti@epfl.ch

Luca Dedè
CMCS-MATHICSE-SB, École Polytechnique Fédérale de Lausanne
Station 8, CH-1015 Lausanne, Switzerland
luca.dede@epfl.ch

Alfio Quarteroni
CMCS-MATHICSE-SB, École Polytechnique Fédérale de Lausanne
Station 8, CH-1015 Lausanne, Switzerland
alfio.quarteroni@epfl.ch

In this talk, we consider the coupling of electrophysiology and mechanical models to realize an integrated model of the left ventricle by considering the active contraction of the muscle and the feedback on the electrophysiology; for the latter, we consider the monodomain equations with the Bueno-Orovio ionic model [1]. As for the solid mechanics of the muscle, we consider the Holzapfl-Ogden model [2] together with an active strain approach [3] with a transmurally variable activation parameter. Moreover, we discuss its integration in an FSI framework. We spatially approximate the model by means of the Finite Element method and discuss the properties of different coupling strategies and time discretization schemes. Among these, we consider a fully coupled strategy with a semi-implicit scheme for the time discretization and compare it with staggered algorithms. In order to solve the large linear system arising from such discretization, we use a preconditioner based on the FaCSI (Factorized Condensed SIMPLE) concept [4]. We present and discuss numerical results obtained in the HPC framework, including patient-specific left ventricle geometries.

References

[1] Bueno-Orovio, A., and Cherry, E.M., and Fenton, F.H. Minimal model for human ventricular action potentials in tissue. *Journal of Theoretical Biology* 253/3 (2008):544-560.

[2] Holzapfel, G. A., and Ogden R.W. Constitutive modelling of passive myocardium: a structurally based framework for material characterization. *Philosophical Transactions*

of the Royal Society of London A: Mathematical, Physical and Engineering Sciences 367.1902 (2009):3445-3475.

[3] Ambrosi, D., and Arioli, G., and Nobile, F., and Quarteroni, A. Electromechanical coupling in cardiac dynamics: the active strain approach. *SIAM Journal on Applied Mathematics* 71.2 (2011):605-621.

[4] Deparis, S., and Forti, D., and Grandperrin, G., and Quarteroni, A. FaCSI: A block parallel preconditioner for fluid-structure interaction in hemodynamics. *MATHICSE Technical Report*, 13, 2015.

Computational study of the risk of restenosis in coronary bypasses

Bruno Guerciotti
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
bruno.guerciotti@polimi.it

Sonia Ippolito
Radiology Unit, Ospedale L. Sacco
Via G.B. Grassi 74, 20157 Milan, Italy
ippolito.sonia@hsacco.it

Alfio Quarteroni
SB MATHICSE CMCS, EPFL
Av. Piccard, Bat. MA, Sec. B2-C2, Station 8, CH-1015 - Lausanne Switzerland
alfio.quarteroni@epfl.ch

Roberto Scrofani
Cardiosurgery Unit, Ospedale L. Sacco
Via G.B. Grassi 74, 20157 Milan, Italy
scrofani.roberto@hsacco.it

Christian Vergara
Politecnico di Milano
Piazza Leonardo da Vinci 32, 20133 Milan, Italy
christian.vergara@polimi.it

Coronary artery disease, which is one of the leading causes of death in the world, is caused by the build-up of atherosclerotic plaques in the vessel walls. The result is a reduction of oxygen supplies to the heart, which increases the risk of myocardial infarction, stroke and unstable angina [1]. For high-risk patients, coronary artery bypass graft (CABG) is the preferred treatment. In particular, the gold standard procedure for the surgical treatment of the left anterior descending (LAD) coronary artery disease is the left internal mammary artery (LIMA) bypass. Despite its excellent patency rates of nearly 90% at 15 years, LIMA bypass may fail due to restenosis. Specifically, the long-term patency of LIMA is thought to be related to the degree of stenosis in the native vessel [2]. In this context, we present a computational study of the fluid-dynamics in patient-specific geometries with the aim of investigating a possible relationship between coronary stenosis and LIMA graft failure. Firstly, we propose a strategy to prescribe realistic boundary conditions in absence of measured data, based on an extension of the well–known Murray's law [3] to provide the flow division at bifurcations in case of stenotic vessels and non--Newtonian blood rheology. With the aim of investigating the actual influence of non-Newtonian blood rheology on the hemodynamics of 3D patient-specific stenotic vessels, we also show some results regarding the comparison between

Newtonian and non-Newtonian rheology. Then, we show the results regarding numerical simulations in patients treated with grafts in which the degree of coronary stenosis is virtually varied, in order to compare the fluid-dynamics in terms of hemodynamic indices potentially involved in restenosis development. Finally, we present some preliminary results concerning fluid-structure interaction simulations in CABGs with the aim of better understanding the influence of the bypass mechanical properties on the risk of graft failure.

References

[1] Beltrame J. F., Dreyer R., Tavella R. S. 2012, *Coronary Artery Disease - Current Concepts in Epidemiology, Pathophysiology, Diagnostics and Treatment*. InTech.

[2] Meng X., Fu Q., Sun W., Yu J., Yue W. and Bi Y. 2013, *Competitive flow arising from varying degrees of coronary artery stenosis affects the blood flow and the production of nitric oxide and endothelin in the internal mammary artery*. Eur. J. Cardio-Thorac. 43, 1022–1027.

[3] Murray C. D. 1926, *The physiological principle of minimum work*. Proc. Natl. Acad. Sci. 12, 207–214.

Mathematical and numerical modeling of heart functioning and systemic circulation - Part III

PROPOSERS

Luca Dedé
Chair of Modelling and Scientific Computing, MATHICSE, École Polytechnique Fédérale de Lausanne
Av.Piccard, Station 8, CH-1015 Lausanne, Switzerland
luca.dede@epfl.ch

Andrea Manzoni
Chair of Modelling and Scientific Computing, MATHICSE, École Polytechnique Fédérale de Lausanne
Av.Piccard, Station 8, CH-1015 Lausanne, Switzerland
andrea.manzoni@epfl.ch

Simone Scacchi
Dipartimento di Matematica, Università di Milano
Via Saldini, 50, 20133 Milano, Italy
simone.scacchi@unimi.it

Christian Vergara
MOX, Dipartimento di Matematica, Politecnico di Milano
Piazza Leonardo da Vinci 32, 20133 - Milano Italy
christian.vergarai@polimi.it

SPEAKERS

Luca F. Pavarino
Department of Mathematics, University of Milano, Italy
luca.pavarino@unimi.it

Luca Gerardo-Giorda
Basque Center for Applied Mathematics, Bilbao, Spain
lgerardo@bcamath.org

Anna Pandolfi
Politecnico di Milano
anna.pandolfi@polimi.it

Damiano Lombardi
REO, INRIA, Paris, France
damiano.lombardi@inria.fr

Lara Charawi
Dipartimento di Matematica, Università di Pavia, Italy
lara.charawi@unimi.it

Diana Bonomi

MOX, Dipartimento di Matematica, Politecnico di Milano, Italy
diana.bonomi@polimi.it

Cardiac and Cardiovascular Mathematics represents nowadays a challenging topic in view of the emerging and growing collaborations between clinicians and mathematicians. In this respect, the numerical solution of problems arising in modeling cardiac and systemic phenomena opens new and interesting perspectives which need to be properly addressed. From the cardiac side, a fully integrated heart model represents a complex multiphysics problem, which is in turn composed of several submodels describing cardiac electrophysiology, mechanics, and fluid dynamics. Each submodel exhibits a spatial and temporal multiscale behavior and poses significant mathematical, numerical and computational challenges. While the systemic circulation has been studied for a longer time, several mathematical and numerical aspects still need to be addressed, as e.g. tissue remodeling, atherosclerotic plaque formation, aneurysms development, transitional and turbulence phenomena in blood flows. This minisymposium aims at gathering researchers and experts in mathematical and numerical modeling of the heart and the systemic circulation at large. Topics include, but are not limited to cardiac models, including electrophysiology, mechanical activation, fluid dynamics of the heart, valve modeling, patient-specific and image-based simulations, as well as fluid-structure interaction in real and large vessels, turbulence models, tissue growth and remodeling.

Parallel simulations of 3D cardiac electro-mechanical models and reentry dynamics

Luca F. Pavarino
Università degli Studi di Milano
via Festa del Perdono, 7 20122 - Milano Italy
luca.pavarino@unimi.it

Piero Colli Franzone
Università degli Studi di Pavia
via Ferrata, 5 27100 Pavia, Italy
colli@imati.cnr.it

Simone Scacchi
Università degli Studi di Milano
via Festa del Perdono, 7 20122 - Milano Italy
simone.scacchi@unimi.it

Cardiac arrhythmias have been studied extensively in the last decades, mostly by employing simplified bioelectrical models on fixed domains without myocardial deformation. The aim of this work is to extend these studies by using multi-physics electro-mechanical models that include the coupling of cardiac bioelectrical and mechanical activities. The main four components of these models are: the quasi-static transversely isotropic finite elasticity equations for the deformation of the cardiac tissue; the active tension model for the intracellular calcium dynamics and cross-bridge binding; the anisotropic Bidomain model for the electrical current flow through the tissue; the membrane model of ventricular myocytes, including stretch-activated channels. In order to properly consider the mechano-electric feedbacks (MEFs), the electrical current flow is described by the Bidomain model on the deformed tissue. The numerical simulations are based on our finite element parallel solver, which employs Multilevel Additive Schwarz preconditioners for the solution of linear systems arising from the discretization of the Bidomain equations and Newton-Krylov-Algebraic Multigrid methods for the solution of the nonlinear systems arising from the discretization of the finite elasticity equations. The simulation results indicate that MEF has a prominent influence on the cardiac repolarization process and should be properly taken into account in simulation studies of cardiac arrhythmias and reentry phenomena.

References

[1] P. Colli Franzone, L.F. Pavarino, S. Scacchi, Bioelectrical effects of mechanical feedbacks in a strongly coupled cardiac electro-mechanical model. Math. Mod. Meth. Appl. Sci. 26 (1): 27-57, 2016.

[2] P. Colli Franzone, L.F. Pavarino, S. Scacchi, Parallel multilevel solvers for the cardiac electro-mechanical coupling. Appl. Numer. Math., 95: 140 – 153, 2015.

A computational model for endocardial radiofrequency ablation with open-irrigated electrode

Luca Gerardo-Giorda
BCAM – Basque Center for Applied Mathematics
Bilbao, Spain
lgerardo@bcamath.org

Ana Gonzalez Suarez
BCAM – Basque Center for Applied Mathematics
Bilbao, Spain
agonzalezs@bcamath.org

Jose M. Guerra
Hospital de la Santa Creu i Sant Pau
Barcelona, Spain
jguerra@santpau.cat

Radiofrequency ablation (RFA) is a common procedure in cardiac catheterization for the treatment of cardiac arrhythmias. Although globally a pretty safe procedure, it may present some risk. Thrombus formation can occur during RFA at the electrode-tissue interface when the temperature exceeds 80ºC. Open-irrigated electrodes have been developed to reduce the risk of thrombus formation by cooling the electrode-tissue interface, allowing higher RF power delivery and the creation of larger lesions. On the other hand, higher RF power delivery increases the risk of steam pops occurrence, a rather serious complication. Steam pops are caused by tissue overheating above 89ºC, and may trigger explosive rupture of myocardium. If the steam pop occurs sufficiently deep in the tissue, or if the RFA is performed on atria, whose walls are thinner that the ones of the ventricles, such explosive rupture may actually result in a perforation of the cardiac chamber wall, and in dramatic hemorrhagic events. As of today, it is still very complicated to predict the occurrence and location of steam pops into the tissue during RFA. We present here a three-dimensional model for catheter RFA with open-irrigated electrode, its validation against in vitro experiments, and show its potential for accurate spatio-temporal prediction of steam pop occurrence.

References

[1] A. Gonzalez Suarez, E. Berjano, J.M. Guerra, and L. Gerardo-Giorda (2016) *Computational Modeling of Open-Irrigated Electrodes for Radiofrequency Cardiac Ablation Including Blood Motion-Saline Flow Interaction.* PLoS ONE 11(3): e0150356. doi:10.1371/journal.pone.0150356.

[2] A. Gonzalez Suarez, E. Berjano, J.M. Guerra, and L. Gerardo-Giorda (2016) *A Computational Model of Open-irrigated Electrode for Endocardial RF Catheter Ablation.*

Computing in Cardiology 42 (2015) 73-76

Electro-mechanical modeling of cardiac tissue considering time-dependent spatially distributed fibers

Anna Pandolfi
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano, Italy
anna.pandolfi@polimi.it

Alessio Gizzi
Università Campus Bio-Medico di Roma
Via A. del Portillo 21, 00128 - Roma, Italy
a.gizzi@unicampus.it

Marcello Vasta
Università di Chieti-Pescara
Viale Pindaro 42 - Pescara, Italy
mvasta@unich.it

Cardiac tissue belongs to the class of excitable deformable biological media undergoing large deformations. Thermodynamics sound frameworks have been recently proposed tacking into account the mechano-electric feedback for sets of deterministic fiber-reinforced structures [1, 2]. The ventricular wall, however, is characterized by a non deterministic distribution of the fiber orientation [3] requiring the adoption of suitable statistical descriptors [4, 5].
In the present contribution we discuss analytical and numerical tools conjugating the statistical characterization of the anisotropic strain energy density of soft hyperelastic materials embedding distributed sets of reinforcing fibers into an electro-active framework. We base our formulation on the classical exponential form of the anisotropic strain energy function, described in terms of the modified invariants of the deformation. We adopt the additive decomposition of the Helmholtz free energy density in elastic and active parts, accompanied to a multiplicative decomposition of the deformation gradient in which we introduce a statistical constitutive prescription for the active deformation gradient tensor.

References

[1] Nobile, F., Quarteroni, A., Ruiz-Baier, R. *An active strain electromechanical model for cardiac tissue*. Int. J. Num. Meth. Biomed. Eng. **28**:52–57, 2012.

[2] Gizzi, A., Cherubini, C., Filippi, S., Pandolfi, A. *Theoretical and numerical modeling of nonlinear electromechanics with applications to biological active media*. Comm. Comput. Phys. **17**:93–126, 2015.

[3] Sommer, G., Schriefl, A.J., Andrä, M., Sacherer, M., Viertler, C., Wolinski, H., Holzapfel, G.A. *Biomechanical properties and microstructure of human ventricular myocardium*. Acta Biomat. **24**:172–192, 2015.

[4] Gasser, T.C., Ogden, R.W., Holzapfel, G.A. *Hyperelastic modeling of arterial layers with distributed collagen fibre orientations.* J. Roy. Soc. Interface **3**:15–35, 2006.

[5] Pandolfi, A., Vasta, M. *Fiber distributed hyperelastic modeling of biological tissues.* Mech. Mat. **44**:151–162, 2012.

Uncertainty quantification on systemic networks: application to clinical monitoring of hypertension

Damiano Lombardi
Inria Paris
2, rue Simone Iff, 75012 Paris
damiano.lombardi@inria.fr

Jean-Frédéric Gerbeau
Inria Paris
2, rue Simone Iff, 75012 Paris
jean-frederic.gerbeau@inria.fr

The clinical monitoring of hypertension is based on the direct measurement of the systemic pressure during the day as well as the assessment of the vessels stiffness by the measurement of the Pulse Wave Velocity (PWV) (see [3] for a review of the guidelines). The latter is the pressure wave speed, that is influenced by the vessels stiffness and varies significantly from the central portion of the cardiovascular system to the periphery. The main goal is to assess the aorta stiffness, in particular close to the heart, possibly in a non-invasive way. Several medical devices are available in order to perform this task. Mathematical modelling can help in understanding the dynamics of the systemic circulation and enrich the available measurements. Models of global circulation are often reduced to a system of 1D hyperbolic equations on networks (In [1] a detailed derivation is proposed). The large number of free parameters which cannot be all identified based on the available set of data (see [2] as an example of sequential approach for parameter estimation) make detailed models of 1D global circulation of little (or questionable) use for an effective clinical monitoring of hypertension. A different approach is investigated, based on an uncertainty quantification formulation of the 1D models on systemic networks. Most of the (unidentifiable) parameters describing the properties of the network are supposed to be random variables, whose priors are set based on the medical knowledge and experimental correlations. The goal is to try to reproduce the daily fluctuations of the cardiovascular activity and match as precisely as possible an available set of data. The byproduct of the model is an assessment of the vessel stiffness that can be more intrinsic than the measurement of the PWV. A preliminary study on realistic data is proposed.

References

[1] Formaggia, L., Quarteroni, A., Veneziani, L. 2009 *Cardiovascular Mathematics* Springer.

[2] Lombardi, D. *Inverse problems in 1D haemodynamics on systemic networks: a sequential approach* International Journal for Numerical Methods in Biomedical Engineering, 2013.

[3] ESH, ESC *Guidelines for the management of arterial hypertension.* Journal of Hypertension, 2007.

Isogeometric Parallel Solvers for the Bidomain System in Electrocardiology

Lara Charawi
Department of Mathematics, Università degli Studi di Pavia
via Ferrata, 1 27100 - Pavia Italy
lara.charawi@unipv.it

We present and study domain decomposition methods for the isogeometric discretization of the reaction-diffusion system which describes the spread of the electrical impulse in the myocardium, the so-called Bidomain model [1]. The cardiac Bidomain model consists of a system of a non-linear parabolic reaction-diffusion partial differential equation (PDE) and an elliptic linear PDE. The evolution equation is coupled through the non-linear reaction term with a stiff system of ordinary differential equations, modeling the ionic currents through the cellular membrane. The different space and time scales involved make the numerical solution of this problem very challenging. We consider Isogeometric Analysis [2] in the framework of the Galerkin method for the spatial approximation of the model and a semi-implicit adaptive method in time. The multilevel overlapping Schwarz preconditioner is applied with a PCG accelerator to solve the linear system arising from the discretization. The resulting solver is scalable, optimal in the ratio of subdomain/element size and the convergence rate improves with increasing overlap size. Parallel numerical tests on an idealized human left ventricle geometry described by NURBS, including intramural fiber rotation and anisotropic conductivity tensor, show the good convergence properties.

References

[1] P. Colli Franzone, L. F. Pavarino and S. Scacchi: *Mathematical cardiac electrophysiology*, Springer MS&A, 2014.

[2] J. A. Cottrell, T. J. R. Hughes and Y. Bazilevs: *Isogeometric analysis: toward integration of CAD and FEA*, John Wiley & Sons, 2009.

Reduced-order models for the efficient solution of the cardiac electromechanical problem

Diana Bonomi
MOX, Dipartimento di matematica, Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
diana.bonomi@polimi.it

Andrea Manzoni
CMCS-MATHICSE-SB, Ecole Polytechnique Fédérale de Lausanne
Station 8, CH-1015 Lausanne, Switzerland
andrea.manzoni@epfl.ch

Alfio Quarteroni
CMCS-MATHICSE-SB, Ecole Polytechnique Fédérale de Lausanne
Station 8, CH-1015 Lausanne, Switzerland
alfio.quarteroni@epfl.ch

We present a reliable and efficient reduced-order framework capable to speed up the solution of coupled parametrized electromechanical problems, aiming at the description of heart functioning in different scenarios.
The need for reduction arises from the increasing interest in understanding how cardiac diseases affect the heart contraction and the propagation of the electrical signal. To do this, we describe the interaction of the cardiac electrophysiology system with the contractile muscle tissue, including the sub-cellular activation-contraction mechanism, see [8] for a detailed review of these aspects. The resulting coupled problem is extremely complex and computationally demanding. For instance, electrical and mechanical models are characterized by different spatial and temporal scales, the former requiring finer computational grids and smaller timesteps, leading to unavoidable high computational costs. Moreover, in order to correctly describe the myocardium, we need a complex nonlinear constitutive law, accounting for the presence of muscular fibers and sheets.
In this respect, we consider the electromechanical model described in [10]. The latter resorts to the monodomain equations [4] coupled to a Bueno-Orovio ionic model [1] to describe the electrical signal propagation. For the mechanical components, we rely on the hyperelastic model proposed by Holzapfel and Ogden [6], which has been widely accepted for the description of the myocardium activity.
Our approach relies on a reduced basis (RB) method [9] that consists in projecting the problems to be solved onto low-dimensional spaces, obtained using the Proper Orthogonal Decomposition technique (POD) [5]. In order to efficiently handle nonlinear terms, we adopt suitable hyper-reduction techniques, for both the electrophysiology and the mechanical subproblems. In particular, the Discrete Empirical Interpolation Method (DEIM) [3] and its matrix version MDEIM [7] are exploited to perform system approximation at a purely algebraic level. In addition, we propose a suitable way to combine solution-space reduction and system approximation, yielding reduced order models able to provide a fast and reliable approximation to the high-fidelity problem, achieving a speed-up of about

two order of magnitude [2].
We present and discuss some numerical results by considering both idealized and patient-specific left ventricle geometries for which we highlight the effectiveness of the proposed method.

References

[1] Bueno-Orovio, A., Cherry, E., Fenton, F., 2008 Minimal model for human ventricular action potentials in tissue. Journal of Theoretical Biology 253(3), 544–560

[2] Bonomi, D., Manzoni, A., Quarteroni, A., *A matrix discrete empirical interpolation method for the efficient model reduction of parametrized nonlinear PDEs: application to nonlinear elasticity problems.* Submitted, Mox Report 14-2016

[3] Chaturantabut, S., Sorensen, D., 2010 Nonlinear Model Reduction via Discrete Empirical Interpolation. SIAM Journal on Scientific Computing 32(5), 2737–2764

[4] Colli Franzone, P., Pavarino, L., Scacchi, S., 2014 *Mathematical cardiac electrophysiology.* Modeling, Simulation and Applications (MS&A) Series, Springer-Verlag Italia, vol. 13.

[5] Everson, R., Sirovich, L., 1995 *Karhunen-Loeve procedure for gappy data.* Journal of the Optical Society of America 12(8)

[6] Holzapfel, G., Ogden, R., 2009 *Constitutive modelling of passive myocardium: a structurally based framework for material characterization.* Philosophical transactions. Series A, Mathematical, physical, and engineering sciences 367(1902), 3445–3475

[7] Negri, F., Manzoni, A., Amsallem, D., 2015 *Efficient model reduction of parametrized systems by matrix discrete empirical interpolation.* J. Comp. Phys. 303, 431–454

[8] Quarteroni, A., Lassila, T., Rossi, S., Ruiz-Baier, R., *Integrated heart - coupling multiscale and multiphysics models for the simulation of the cardiac function.* Submitted, Mox Report 05-2016

[9] Quarteroni, A., Manzoni, A., Negri, F., 2016 *Reduced Basis Methods for Partial Differential Equations. An Introduction.* Unitext, vol. 92. Springer

[10] Rossi, S., Lassila, T., Ruiz-Baier, R., Sequeira, A., Quarteroni, A., 2013 *Thermodynamically consistent orthotropic activation model capturing ventricular systolic wall thickening in cardiac electromechanics.* European Journal of Mechanics, A/Solids 48

Algebraic Techniques & Graphs Theory to Analyse-Design Estimation-Prediction Dynamic Systems

PROPOSERS

Mario Versaci
Università degli Studi di Reggio Calabria
via Graziella Feo di Vito, 89122 - Reggio Calabria, Italy
mario.versaci@unirc.it

SPEAKERS

Mario Versaci
Università degli Studi di Reggio Calabria
mario.versaci@unirc.it

Vittoria Bonanzinga
Dept. DIIES, Universitá di Reggio Calabria
vittoria.bonanzinga@unirc.it

Gioia Failla
Dept. DIIES, Universitá di Reggio Calabria
gioia.failla@unirc.it

Maurizio Imbesi
Dept. of Mathematics Informatics and Earth Sciences, Universitá di Messina
maurizio.imbesi@unime.it

Gaetana Restuccia
Dept. of Mathematics Informatics and Earth Sciences, Universitá di Messina
tania.restuccia@gmail.com

In industrial domain, analysis and design of dynamic processes by Artificial Neural Networks (ANNs) are considered as a strategical focus because allow, on the one hand, the modelization of both estimation and prediction problem by graphs and, secondly, easier possibility for updating of the performances by optimization techniques with an acceptable computational complexity useful for real-time applications [1]. However, to reduce CPU-time and to allow optimal performances, it is necessary to build ANNs with both a reduced number of inputs and to be connected and complete respectively (Fig.1). In such a context, it develops the idea of proposing this Minisymposium with the intent to disseminate the ACCA &AP SIMAI Group activities to which the Speakers belong. In particular, the Group, albeit working synergically to achieve the aims as set out above, is working on several fronts.

The first one, purely algebraic, works on the ranking of the input data: a set of data can be studied ranking them following criteria suggested from the problem. A classical model describing the ranking is the Birkoff model and the Birkoff polytope. We take interest in what happens to submodels of the Birkoff model and corrensponding

subpolytopes. In the description of each model the theory of Groebner bases is very crucial [2]. The second one, geometrically, acts on both the investigation of the connection and completeness of graphs of lattice points inside the Segre-Veronese model [3] and on the chord length distribution for non convex polygons [4]. The aim of the third one deals with dynamic models to simulate inputs-outputs mapping as well as to evaluate ANNs able to distinguish the impact of some modeling parameters on specific and peculiar features when both estimation and prediction problems are taken into account.

References

[1] Cacciola, M., La Foresta, F., Morabito, F.C., Versaci, M., Neural Networks for the Parameters Characterization of ECG Dynamical Model, New Dir. in Neural Nets, IOS Press, 2009, 40 – 49.

[2] Sturmfels, B., Gröbner Bases and Convex Polytopes, University Lecture Series, 8, Amer. Math. Soc., Providence, RI, 1996.

[3] Failla, G., Utano, R., Connected Graphs Arising from Products of Veronese Varieties, Algebra Colloquium 23:2 (2016) 281–292 DOI: 10.1142/S1005386716000304.

[4] Duma, A., Rizzo, S., Chord lenght distribution function for an arbitrary triangle, Suppl. Rend. Circ. Mat. Palermo, Serie II 81, 2009, pp 141–157.

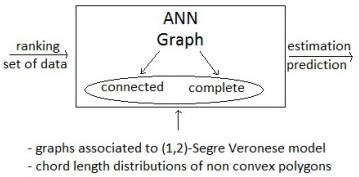


Figure 1: ACCA &AP SIMAI Group activities synergies

An Algebraic Soft Computing Approach to Solve Prediction Problems in Artificial Neural Networks Domain (ANNs)

Mario Versaci
DICEAM, Universitá *Mediterranea* di Reggio Calabria
via Graziella - Loc. Feo di Vito, 89121 - Reggio Calabria Italy
mario.versaci@unirc.it

Giovanni Angiulli
DIIES, Universitá *Mediterranea* di Reggio Calabria
via Graziella - Loc. Feo di Vito, 89121 - Reggio Calabria Italy
giovanni.angiulli@unirc.it

In industrial context, design and analysis of dynamical processes $y = f(x)$ by ANNs have a crucial role because allow, firstly, the modelization of both the estimation and prediction problems by algebraic approaches and, secondly, easier possibility for updating of the performances by optimization techniques with a reduced computational complexity so useful for real-time applications (low CPU-time). Nevertheless, industrial processes could be characterized by uncertainty and/or vagueness so it is imperative to take into account suitable techniques, such as fuzzy ones, to treat this eventuality at hand. Matematically, focusing the attention on algebraic prediction systems by means of two factors fuzzy time series, $y(t)$ represents a one-dimensional time observations represented by crisp values. If $y(t)$, the so-called main factor, represents a set of real number, then $b(t)$, a collection of $f_i(t)$ (set of membership functions defined on Y ranging over $[0, 1]$), represents a fuzzy time series of $y(t)$ (secondary factor). Once Y and B, the compact Universes of Discourse of $y(t)$ and $b(t)$ respectively have been built, the fuzzification process will be based on the variation of both the main and secondary factors. If, at time t, $b(t)$ is caused by $b(t-1)$, their fuzzy relationship can be written by $b(t) = b(t-1) \cdot M(t, t-1)$. In order to built matrix M, it is necessary to make a criterion vector $CV(t)$ and an operational matrix $O(t)$ (depending on the time window) so that the Cheng's approach, a sort of product among $O(t)$, $CV(t)$ and $T(t)$ (fuzzification of the secondary factor), can be applied. Conceptually, defuzzification procedure is quite because based on the following supposition in terms of fuzzy rule structure:
"**IF** membership value of predicted variation=0 **THEN** predicted variation =0 **ELSE IF** maximum membership value of fuzzified predicted variation=0 **THEN** predicted variation=midpoint (t)."
The proposed procedure was applied to the prediction fo the intracranial pressure values of patients suffering from brain cancer. The obtained results can be considered encouraging if compared with the results carried out by established techniques.

References

[1] Versaci M, Morabito F.C., 2003 *Fuzzy Time Series Approach for Disruption Prediction in Tokamak Reactors*, IEEE Transaction on Magnetics, Vol. 39, pp. 1503-1506.

[2] Lee M.H., Suhartono M. et al., 2012 *Fuzzy Time Series: an Application to Tourism Demand Forecasting*, American Journal of Applied Scienes, Vol. 9, pp. 132-140.

Chord length distributions of non convex polygons with applications to telecommunication networks

Vittoria Bonanzinga
Università degli Studi di Reggio Calabria
via Graziella, Feo di Vito, 89100 - Reggio Calabria Italy
vittoria.bonanzinga@unirc.it

Uwe Bäsel
HTWK Leipzig, University of Applied Sciences,
Faculty of Mechanical and Energy Engineering, PF 30 11 66, 04251 Leipzig, Germany
uwe.baesel@htwk-leipzig.de

Andrei Duma
FernUniversität in Hagen
Fakultät Mathematik und Informatik 58084 Hagen, Germany
mathe.duma@FernUni-Hagen.de

The chord length distribution functions of several plane convex figures are already known. We refer to the following results:

- regular hexagon [4],
- rectangle [10],
- arbitrary triangle [5], [3],
- rectangular trapezium [6],
- isosceles trapezium [12],
- every regular polygon [8], [2].

In 2011, Barilla, Duma and Puglisi studied the distribution function of the chord length of a non convex polygon [1]. The distribution function of the distance between two uniformly and independently distributed random points in every regular polygon is derived in [2]. In this work, we calculate the chord length distribution function and the corresponding density function of a non convex, equilateral hexagon. The chord length distributions have practical applications in different fields: in physics, for instance in small angle scattering SAS [3], [7], in chemistry, for instance in the characterization of random composite and porous materials [11], and in communication engineering, in random networks, as wireless mobile systems such as cellular and sensor networks [9], [13].

References

[1] Barilla, D., Duma, A., and Puglisi, A. 2011 *The distribution function of a chord in a non convex polygon.* Suppl. Rend. Circ. Mat. Palermo, Serie II, 83, 23–40.

[2] Bäsel, U., 2014. *Random chords and points distances in regular polygons.* Acta Math. Univ. Comenianae, Vol. 83, 1–18.

[3] Ciccariello, S., 2010. *The isotropic correlation function of plane figures: the triangle case.* Journal of Physics: Conference Series 247, 012014, XIV International Conference on Small-Angle Scattering (SAS09), 1–10.

[4] Conserva, V., Duma, A., 2007 *Schnitte eines regulären Hexagons in Buffon- und Laplace-Gitter.* Hagen, Band 78, 29–36.

[5] Duma., A., Rizzo, S., 2009. *Chord length distribution function for an arbitrary triangle.* Suppl. Rend. Circ. Mat. Palermo, Serie II, 81, 147–160.

[6] Duma., A., Rizzo, S., 2011. *La funzione di distribuzione di una corda su un trapezio rettangolo* Suppl. Rend. Circ. Mat. Palermo, Serie II, 83, 141–157.

[7] Gille., W., 2014 *Particle and Particle Systems Characterization: Small-Angle Scattering (SAS) Applications.* CRC Press, Boca Raton/London/New York.

[8] Harutyunyan, H. S., Ohanyan, V. K., 2009, *The chord length distribution function for regular polygons.* Adv. in Appl. Probab., Volume 41, Number 2, 358-366.

[9] Moltchanov, D. 2012 *Survey paper: Distance distributions in random networks.* Journal Ad Hoc Networks, 10, 6, 1146–1166.

[10] Pettineo, M. 2009 *Geometric probability problems for Buffon and Laplace grid.* Suppl. Rend. Circ. Mat. Palermo, Serie II, 81, 267–274.

[11] Roberts, A. P., Torquato, S., 1999, *Chord-distribution functions of three-dimensional random media: Approximate first-passage times of Gaussian processes.* Physical Review 59, 5, 4953–4963.

[12] Sorrenti, L., 2012, *Chord length distribution functions for an isosceles trapezium.* General Mathematics, 20, 1, 9–24.

[13] Srinivasa, S., Haenggi, M., 2010, *Distance distributions in finite Uniformly Random Networks: Theory and Applications.* IEEE Trans. Veh. Technol. 59, (2), 940–949.

On graphs associated to $(1,2)-$Segre$-$Veronese squarefree model for business

Gioia Failla
DIIES, University of Reggio Calabria
Loc. Feo di Vito, 89122 - Reggio Calabria Italy
gioia.failla@unirc.it

We consider the $(1,2)$-Segre-Veronese squarefree model $A_{(1,2)}$ for a transportation plane of indivisible goods, represented by the Segre product of a polynomial ring $K[x_1,\ldots,x_m]$ in m variables and the 2-nd Veronese squarefree $A^{(2)}$ subalgebra generated by all square free monomials of degree 2 of $K[y_1,\ldots,y_n]$, polynomial ring in n variables.
It is known that to each configuration of lattice points of the affine space, having as support the field K, one associates a family of graphs having as vertices the points of fibers of the semigroup homomorphism f given by the configuration and whose edges are determined by the kernel of f. All such graphs are simultaneously connected if a condition on the Groebner basis of the toric ideal of the monomial algebra, arising from the lifting of the homomorphism of semigroups, is verified.
We investigate the problem for the special configuration given by $A_{(1,2)}$.
In previous papers we studied the Groebner basis of the toric ideal $I_{(1,2)}$ of the monomial algebra $A_{(1,2)}$.
It is quadratic for a special term order so called sorted order and it consists only of the generators of $I_{(1,2)}$.
An open problem is to find graphs inside the family that are bipartite or having good properties, as completeness. We study

1. the graphs associated to the configuration of $A^{(2)}$
2. the graphs associated to the the configuration of $A_{(1,2)}$

In particular the graphs having as support the kernel of f (the fiber of the zero of $A_{(1,2)}$) is investigated for low values of m and n. The interpretation in terms of the transportation plan is given.

References

[1] Failla, G. 2014 *On the* $(1,1)$*-Segre Model for Business*, Applied Mathematical Sciences, Vol.8, n.166, 8329-8336

[2] Failla, G., Utano R. 2016 *Connected graphs arising from products of Veronese varieties*, Algebra Colloquium, 23, n.2,281-292

[3] Sturmfels, B 1995 *Groebner bases and convex polytopes*, Univ.Lect.Series, Vol.8, Amer.Math.Soc

Graph representation for the blow up of $\mathbb{P}^2$ at some points

Maurizio Imbesi
Università degli Studi di Messina
Viale F. Stagno d'Alcontres, 31 98166 - Messina Italy
imbesim@unime.it

Mustapha Lahyane
Universidad Michoacana de San Nicolás de Hidalgo
Avenida Francisco J. Múgica s/n 58040 - Morelia México
lahyane@ifm.umich.mx

The geometry of projective varieties offers a strong tool for solving efficiently problems coming from different areas; for instance in coding theory, it allows to get algebraic-geometric codes with very good parameters and whose applications to the real life greatly changed human styles of life, see the references [1, 2] among so many.

We will take into account Harbourne's basic rational surfaces over an algebraically closed field k of any characteristic, concretely these are all the smooth projective rational surfaces obtained as the blow up of $\mathbb{P}^2_k$ at a finite number of points not necessarily in general position.

The geometry of a basic rational surface X is encoded in its effective monoid $\mathrm{Eff}(X)$ which consists of the set of effective elements of the Néron-Severi group $\mathrm{NS}(X)$ of X, namely the quotient group of the group of Cartier divisors on X modulo the numerical equivalence. $\mathrm{NS}(X)$ is a free $\mathbb{Z}$-module whose rank, denoted by $\rho(X)$, is called the Picard number of X.

For a generic rational surface X with $\rho(X) \geq 10$, Nagata proved that $\mathrm{Eff}(X)$ is not finitely generated. The basic rational surfaces with Picard number less than 10 are obtained as the blow up of $\mathbb{P}^2_k$ at r points, with $r \leq 8$; in fact, using Nagata's result, if we consider the blow up of $\mathbb{P}^2_k$ at least at 9 points in general position, its effective monoid is not finitely generated because this surface has an infinity number of (-1)-curves. Nowadays, it is well-known that the effective monoid of the blow up of $\mathbb{P}^2_k$ at most at 8 points is finitely generated; a minimal generating set of it in the generic case is computed for example in [3].

However up to now, there is not a complete list for the effective monoids of such rational surfaces, neither a convenient one in the case of the generic situations. Our goal is to apply smoothly graph theory in order to lead to an entire classification of them; precisely, we will be able to connect the blow ups that have finitely generated effective monoids to well-determined weighted graphs both when the points are in general position and when they are collinear or infinitely near, even drawing an exhaustive representation of such graphs.

It is evident to realize what numberless applications could derive in contexts so varied as communication networks, interchange systems, sensitive data transmission and so on by simply pointing out the several kinds of the obtained weighted graphs.

References

[1] Goppa, V.D. 1982 *Algebraic-geometric codes.* Izv. Akad. Nauk SSSR Mat. 46, 4, 762–781.

[2] Hansen, S.H. 2001 *Error-correcting codes from higher-dimensional varieties.* Finite Fields Appl. 7, 4, 531–552.

[3] Rosoff, J. 1980 *Effective divisor classes and blowings-up of* $\mathbb{P}^2$. Pacific J. Math. 89, 2, 419–429.

Ranking problems and Groebner bases

Gaetana Restuccia
Dipartimento di Scienze Matematiche, Informatiche, Scienze Fisiche e Scienze della Terra
Viale Ferdinando D'Alcontres, 31
98166 MESSINA
gaetana.restuccia@unime.it

A set of data can be studied ranking them following criteria suggested from the problem. A classical model describing the ranking allows to the Birkoff model and to the Birkoff polytope. We investigate on submodels of the Birkoff model B_i and on the corresponding subpolytopes. More precisely, in [2], the proper subset of S_n, where S_n is the symmetric group on n elements of cardinality $n!$, consisting of one $n-1$ chain and one incomparable element, is studied. Here we consider more general situations where the subset S' of S_n consists of two chains of lenght $n-i$ and $i, i>1$. The two chains can represent two indipendent lists, based on preferences assigned by multiple voters, inside a unique list for a political team. The elements of the two lists are two to two incomparable under multiple criteria adopted in the specific situation. In the description of each model the theory of Groebner bases is very crucial. We construct before the model , consisting of the polynomial ring $K[X_\pi, \pi \in S']$, and of an homomorphism f into the monomial algebra, a subalgebra of $K[Y_1, ..., Y_n]$ (called the space of the parameters), generated from the images under f. The images are monomials of the same degree. We call the monomial algebra $B'i$, simulating the classical Birkoff model. Then we consider the Groebner basis of the toric ideal of $B'i$ with respect to the lexicographic order but different term orders can be introduced. The corresponding subpolytopes are described and studied. For a few values of $i>1$, we compute all the objects associated to the problem, giving some interpretations.

References

[1] G. Restuccia, Algebraic models in different fields, Applied mathematical sciences, Vol. 8, 2014, n. 167,8345-8351

[2] B. Sturmfels, Groebner bases and convex polytopes, Univ. Lect. Series, Vol. 8, Amer. Math. Soc., 1995

Small–scale Solid and Fluid Mechanics in Biology - Part I

PROPOSERS

Davide Ambrosi
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
davide.ambrosi@polimi.it

Paolo Zunino
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
paolo.zunino@polimi.it

SPEAKERS

Antonio DeSimone (keynote)
SISSA
antonio.desimone@sissa.it

Giuseppe Sciumè
Università del Salento
giuseppe.sciume@unisalento.it

Alberto García
Politecnico di Milano
alberto.garcia@polimi.it

Alessandro Musesti
Università di Brescia
alessandro.musesti@unicatt.it

Abramo Agosti
Politecnico di Milano
abramo.agosti@polimi.it

The minisymposium aims to gather the italian community of scientists working on the mathematical modelling and numerical simulation of mechanobiology at a tissue scale, with an emphasis on the biomedical perspective. Specific issues of interest will be the microcirculation, the growth of malignant tissues, the cellular and subcellular mechanics, nanomedicine and muscles. Both experimental, modeling and numerical methodologies will be tackled.

Locomotion at microscopic scales: some case studies on biological and bio-inspired motility

Antonio DeSimone
SISSA–International School for Advanced Studies
via Bonomea 265, 34136 - Trieste Italy
desimone@sissa.it

Giovanni Noselli
SISSA–International School for Advanced Studies
via Bonomea 265, 34136 - Trieste Italy
gnoselli@sissa.it

Motility of cells, whose typical size is in the tens of micrometers, is at the root of many fundamental processes in Biology. These include the immune system response, the establishment of connections in the nervous system network, metastatic tumour cells crawling to invade nearby tissues, and sperm cells successfully swimming their way by beating a flagellum until they reach and fertilise an egg cell. The detailed understanding of the mechanical processes enabling biological locomotion at the micro-meter scale is still a challenge. In addition, motile cells can be regarded as micro-meter-scale, self-sufficient machines capable of executing controlled motion. Their design has been optimised by evolution and natural selection. Learning the mechanical details of how cells move may guide the future design of bio-inspired, motile microscopic devices capable of navigating inside the human body for diagnostic or therapeutic purposes [7, 8, 1]. While the idea of building artificial devices emulating the capabilities of motile cells is quite natural, much remains to be done for this to be practical.

In recent years, we have been studying the mechanical bases of cellular motility by swimming and crawling [3, 6]. In the context of swimming motility, our research has paid special attention on the connections between low Reynolds number swimming and Geometric Control Theory, and on the geometric structure of the underlying equations of motion [3, 6, 2]. The goal of our emphasis on conceptual principles has been the attempt to extract, from the study of the biological template, "recipes" for the successful design of engineered bio-inspired constructs. As a concrete example of our approach, we report on recent progress on reverse engineering of the euglenoid movement [5, 4].

Euglenids are unicellular aquatic organisms capable of moving either by beating a flagellum or by executing dramatic shape changes. These are accomplished thanks to a complex structure underlying the plasma membrane, made of interlocking proteinaceous strips, microtubules, and motor proteins. We discuss the mechanisms by which the sliding of pellicle strips leads to shape control and locomotion, which have been studied by means of both theory (through the mechanics of active surfaces and its coupling to computational fluid dynamics for the surrounding fluid) and experiments. Moreover, we have implemented them into a new concept of surfaces with programmable shape, obtained by assembling 3d-printed strips in a construct mimicking the biological template. We show that the subtle balance between constraints and flexibility leads to a wide variety of shapes that can be obtained with relatively simple controls. This suggests that euglenids

exploit the passive resistance of body parts to reduce the complexity of controlling their shape. This is in close analogy to the notion of "morphological computation", which has been advocated for the design of soft robots inspired by biological systems.

Acknowledgments This research has been funded by the European Research Council under the European UnionÕs Seventh Framework Programme (FP/2007Ð2013)/ERC Grant Agreement No. 340685-MicroMotility (ERC Advanced Grant).

References

[1] F. Alouges, A. DeSimone, L. Giraldi, M. Zoppello 2015: *Can magnetic multilayers propel artificial microswimmers mimicking sperm cells?* Soft Robotics 2, 117–128.

[2] F. Alouges, A. DeSimone, L. Heltai, A. Lefebvre, B. Merlet 2013: *Optimally swimming Stokesian robots*. Discrete Cont. Dyn. Systems B 18, 1189–1215.

[3] F. Alouges, A. DeSimone, A. Lefebvre 2008: *Optimal strokes for low Reynolds number swimmers: an example*. J. Nonlinear Science 18, 277–302.

[4] M. Arroyo, A. DeSimone 2014: *Shape control of active surfaces inspired by the movement of euglenids*. J. Mech. Phys. Solids 62, 99–112.

[5] M.Arroyo, L. Heltai, D. Milan, A. DeSimone 2012: *Reverse engineering the euglenoid movement*. Proc. National Academy of Sciences USA 109, 17874–17879.

[6] A. DeSimone, A. Tatone 2012: *Crawling motility through the analysis of model locomotors: two case studies*. Eur. Phys. J. E 35, article no. 85.

[7] R. Dreyfus et al. 2005: *Microscopic artificial swimmers*. Nature 437, 862–865.

[8] J.Feng and S.K. Cho 2014: *Mini and Micro Propulsion for Medical Swimmers*. Micromachines 5, 97–113.

Mechanobiology of tumor growth: emerging paradigms from mechanics of porous medium systems

Giuseppe Sciumè
University of Bordeaux
I2M - Esplanade des Arts et Metiers 33405 - Talence France
giuseppe.sciume@u-bordeaux.fr

Andreas Bikfalvi
University of Bordeaux
INSERM U1029 - Allee Geoffroy Saint Hilaire Bat. B2, 33615 - Pessac France
andreas.bikfalvi@u-bordeaux.fr

Experimental and clinical cancer research has clearly established that in addition to chemical and biological factors, physical forces have a primary role on tumor growth [1, 3]. Actually, a growing tumor mass is an open thermodynamic system interacting with the host tissue and its vascular and lymphatic systems with which it exchanges mass and energy. Its phenomenology is very complex because several factors coupled each other impact on tumor cells proliferation and this makes mathematical modeling of tumor growth a demanding and challenging task.
A multiphase model for tumor growth during the avascular stage is presented [4-6]. The mathematical formulation has been developed within the framework of Thermodynamically Constrained Averaging Theory (Gray and Miller [2]).
Tumor tissue is modeled as a multiphase system including four phases: the extracellular matrix, ECM, tumor cells, TC (mixture of living and necrotic tumor cells), healthy tissue cells, HC, and interstitial fluid, IF. The ECM is the solid phase of the system and is modeled as a deformable porous continuum, while TC, HC and IF are modeled as immiscible fluid phases. Advection-diffusion of oxygen in IF is also considered, with oxygen assumed being the species having the main impact on cellular metabolism, growth and necrosis.
Examples of biological interest, such as growth of spheroids *in vitro* and *in vivo*, tumor growth in proximity of blood vessels (which generates cell clusters having the shape of a spindle, commonly called tumor cord) and growth of a skin melanoma are presented.
Finally, on ongoing work on modeling of vascular tumor growth is briefly outlined. Modeling of angiogenesis by accounting for blood vessels as a new phase in the porous medium system upgrades the mathematical model for tumor growth during the vascular stage and makes it suitable for simulation of drugs transport/delivery and prediction of tumor response to therapeutic regimens.

References

[1] Ferrari, M. 2010 *Frontiers in cancer nanomedicine: directing mass transport through biological barriers.* Trends in Biotechnology.

[2] Gray, W. G. and Miller, C.T. 2005 *Thermodynamically constrained averaging theory approach for modelling flow and transport phenomena in porous medium systems: 1. Motivation and overview*. Advances in Water Resources.

[3] Michor, F., Liphardt, J., Ferrari, M., Widom J. 2011 *What does physics have to do with cancer?* Nature Reviews Cancer.

[4] Sciumè, G., Shelton, S., Gray, W. G., Miller, C. T., Hussain, F., Ferrari, M., Decuzzi, P., Schrefler, B. A. 2013 *A multiphase model for three-dimensional tumor growth*. New Journal of Physics.

[5] Sciumè, G., Gray, W. G., Hussain, F., Ferrari, M., Decuzzi, P., Schrefler, B. A. 2014 *Three phase flow dynamics in tumor growth*. Computational Mechanics.

[6] Sciumè, G., Santagiuliana, R., Ferrari, M., Decuzzi, P., Schrefler, B. A. 2014 *A tumor growth model with deformable ECM*. Physical Biology

Multiscale Numerical Model of the Strain-Based Permeability of the Nuclear Envelope

Alberto García
Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta"
Politecnico di Milano, Piazza Leonardo da Vinci, 32 20133 - Milano Italy
alberto.garcia@polimi.it

Emanuela Jacchetti
Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta"
Politecnico di Milano, Piazza Leonardo da Vinci, 32 20133 - Milano Italy
emanuela.jacchetti@polimi.it

José Félix Rodríguez Matas
Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta"
Politecnico di Milano, Piazza Leonardo da Vinci, 32 20133 - Milano Italy
josefelix.rodriguezmatas@polimi.it

Manuela Teresa Raimondi
Dipartimento di Chimica, Materiali e Ingegneria Chimica "Giulio Natta"
Politecnico di Milano, Piazza Leonardo da Vinci, 32 20133 - Milano Italy
manuela.raimondi@polimi.it

A basic recent understanding in stem cell differentiation is that the cell is able to translate its shape (e.g. roundish or deformed) into a fate decision. However, the mechanisms by which phenotype expression is regulated by cell shape are complex and poorly understood. Our hypothesis is that cell deformation induces nuclear deformation, which in turn causes strains in the nuclear envelope (NE). These strains cause a change in porosity/permeability of the NE to the traffic of transcription factors involved in stem cell differentiation [1]. To demonstrate this hypothesis, we set-up a numerical model of the interaction between the nuclear pore complexes (NPC) and the NE. It is worth mentioning that the NPC is assumed as a multiprotein structure with a "basket shape" in the nuclear side that plays a significant role in the transport of solutes through the NE [2, 3].

In parallel to the computational modeling and analysis, we recreated in the laboratory the two extreme deformation conditions for the NE by using mesenchymal stem cells (MSC) derived from the bone marrow of adult rat; the cells were seeded and grown on two different substrates: i) a glass flat surface, and ii) a 3D nanoengineered synthetic niche. The flat surface leads to the deformed nuclear configuration, whereas the niche induces the roundish nuclear shape. MSC were incubated at 37^oC with $0.1\mu M$ of Hoechst 3342, a vital and fluorescent little (615 Dalton) molecule, that can freely diffuse inside the cells and bind stably to the DNA. After 10 minutes cells were washed in PBS three times and then placed on a fresh cell culture medium. Samples were mounted into the FluoView10i laser scanning confocal microscope (Olympus) to acquire images (with $30\mu m$ depth and step $1\mu m$) of the cells in both configurations. The nuclear intensity/pixel of each cell is

calculated by manual segmentation of the nuclei and by measurement of the fluorescence intensity of the region of interest.
In order to couple a change in permeability of the NE at the microscale with a change in configuration of a single NPC at the nanoscale (in response to the deformation applied to the NE), we incorporated the measured data of the nuclei main axis from [1] into a computational model of the NPC-NE mechanical interaction. Such experimental measurements were taken inside and outside the aforementioned niches. Considering that the NPC is directly attached to the nuclear lamina, the effect of the nuclear deformation due to mechanotransduction will directly open or close the effective area of the pores, thus increasing or decreasing the permeability of the NE. Here we propose a numerical model that defines the permeability as the areal ratio between the whole nucleus surface area and the total area of the pores. A value of diffusion is then calculated as the product of the permeability and the maximum diffusion coefficient in the cytoplasm (free diffusion) of Hoecst 33342 calculated by means of the Stokes-Einstein law an its molecular weight [4]. Using the continuum mechanics theory for thin lamina, we calculate the pore opening as a function of the local Green-Lagrange deformation tensor at every point on the nuclear surface. We considered an equispaced distribution of NPC's on the NE so that a local permeability is then calculated by dividing the occupied area of a deformed pore by the corresponding NE local area. To do that, we considered the cell as incompressible, that means, the final ellipsoidal volume from [1] will be equal to its corresponding "zero-stress" spherical configuration. Finally, a strain-dependent value of diffusion was calculated and directly applied to a passive transport finite element simulation following the Fick's laws of diffusion.
Our preliminary simulation results show a faster transport of solutes on the deformed NE as compared to the roundish nucleus (a ratio of 7,66:1 faster in the deformed nucleus with respect to the roundish configuration). These results correlate well with experiments performed with Hoecst 33342 where a significantly higher intensity per pixel was found in highly deformed nuclei (cells on the flat surface), suggesting a faster transport through the NE with respect to less deformed nuclei. These results indicate the strain dependence of the passive diffusion process of nucleocytoplasmic transport of solutes. In addition, the computational model is able to recreate such passive transport dependency with respect to the deformation of the nucleus.
This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 646990 - NICHOID).

References

[1] Michele M. Nava, Roberto Fedele, Manuela T. Raimondi 2015 *Computational prediction of strain-dependent diffusion of transcription factors through the cell nucleus.* Biomechanics and Modeling in Mechanobiology, pp 1-11.

[2] Bui et al. 2013 *Integrated structural analysis of the human nuclear pore complex scaffold.* Cell, vol. 155, 1233-1243.

[3] Stoffler et al. 1999 *Calcium-mediated structural changes of native nuclear pores complexes monitored by time-lapse atomic force microscopy.* Journal of Molecular Biology, 287(4), 741-752

[4] Harold P. Erickson 2009 *Size and shape of protein molecules at the nanometer level. determined by sedimentation, gel filtration, and electron microscopy.* Biological Procedures Online, vol. 11, Num. 1.

Loss of performance in skeletal muscle tissue: a continuum model

Alessandro Musesti
Università Cattolica del Sacro Cuore
via dei Musei, 41 25121 - Brescia Italy
alessandro.musesti@unicatt.it

Giulia Giantesio
Università Cattolica del Sacro Cuore
via dei Musei, 41 25121 - Brescia Italy
giulia.giantesio@unicatt.it

Skeletal muscle tissue, whose principal role is the production of *force* and hence *movement*, is a highly-ordered hierarchical structure. Muscular fibres, the cells of the tissue, are organized in fascicles, where every fiber is multiply connected to nerve axons. They contain a concatenation of millions of sarcomers, which are the fundamental unit of the muscle and the actuators of *activation*, the mechanism by which a muscle produces force.
The aim of this contribution is to propose a mathematical model of skeletal muscle tissue with a reduced performance, which is typical of a geriatric syndrome named *sarcopenia* [6]. Sarcopenia is defined as the loss of skeletal muscle mass and strength that occurs with advancing age. Although nowadays the syndrome affects more than 50 millions people, so far there are no compelling tests for its diagnosis and many efforts are made by the medical community to better understand it. Therefore it is desirable to build a mathematical model of muscle tissue affected by sarcopenia.
We will model the tissue as a transversely isotropic and incompressible continuum material. The former assumption is motivated by the alignment of the muscular fibres, while the latter is ensured by the high water content of the tissue. Focusing our attention only on steady properties, we neglect the viscous effects and restrict ourselves to the framework of hyperelasticity. In the model that we propose, there are three constitutive prescriptions: one for the hyperelastic energy when the tissue is not activated (*passive energy*), one for the activation and one for the loss of performance.
As far as the passive part is concerned, we assume an exponential stress response of the material, which is customary in biological tissues. Denoting with $\mathbf{F}$ the deformation gradient and with $\mathbf{C} = \mathbf{F}^T\mathbf{F}$ the right Cauchy-Green tensor, the hyperelastic strain energy density is given by

$$W(\mathbf{C}) = \frac{\mu}{4}\left\{\frac{1}{\alpha}\left[e^{\alpha(I_p-1)} - 1\right] + K_p - 1\right\}, \tag{1}$$

where I_p and K_p are two generalized invariants which account for the isotropic and anisotropic components of the tissue. Here μ is an elastic parameter and α a positive dimensionless material parameter. Such an energy density is a slight simplification of the one proposed in [3]; in particular, it is polyconvex and coercive.
Coming to the activation, a recent and very promising way to describe it is the so called *active strain* approach [2], where the extra energy produced by the activation mechanism

is encoded in a multiplicative decomposition of the deformation gradient in an elastic and an active part:

$$\mathbf{F} = \mathbf{F}_e\mathbf{F}_a.$$

Unlike the classical *active stress* approach, in which the active part of the stress is modeled in a pure phenomenological way and a new term has to be added to the passive energy, the active strain method does not change the form of the elastic energy, keeping in particular all its mathematical properties. Furthermore, in the case of muscles the active strain approach is more adherent to the physiology of the tissue, being a mathematical representation of the contraction of the sarcomeres at the molecular level. The active strain approach has firstly been applied to the skeletal muscle tissue in [4].
Finally, we consider the loss of performance, which is one of the novelties of our model. We model it in two components, both typical of sarcopenia: the loss of muscle mass and the loss of activation. The former is encoded in the model by a percentage parameter g which measures the fraction of muscle fibres which are not active anymore; the latter is represented by a damage parameter d which reduces the active part of the stress by a given percentage. The lack of experimental data on the elastic properties of a sarcopenic muscle tissue does not allow any fitting of the two parameters; however, the proposed model can be numerically implemented using finite element methods and some different scenarios can be studied.
We will present some results obtained using FEniCS [1], an open source collection of Python libraries, showing that the experimental results of [5] on the passive and active stress-strain healthy curves, obtained *in vivo* from a tetanized tibialis anterior of a rat, can be well reproduced by our model in the healthy case. Further, the behavior of the tissue when g and d increase is analyzed.

References

[1] M.S. Alnæs, J. Blechta, J. Hake, A. Johansson, B. Kehlet, A. Logg, C. Richardson, J. Ring, M.E. Rognes, G.N. Wells: The FEniCS Project Version 1.5, Archive of Numerical Software **100**, 9–23 (2015)

[2] D. Ambrosi, S. Pezzuto: Active Stress vs. Active Strain in Mechanobiology: Constitutive Issues. Journal of Elasticity **107**, 199–212 (2012)

[3] A.E. Ehret,M. Böl, M. Itskov: A continuum constitutive model for the active behaviour of skeletal muscle. Journal of the Mechanics and Physics of Solids **59**, 625–636 (2011)

[4] G. Giantesio, A. Musesti: A continuum model of skeletal muscle tissue with loss of activation, in A. Gerisch, R. Penta, J. Lang (Eds), Multiscale Models in Mechano and Tumor Biology: Modeling, Homogenization, and Applications, Springer, submitted

[5] D. Hawkins, M. Bey: A comprehensive approach for studying muscle-tendon mechanics. ASME Journal of Biomechanical Engineering **116**, 51–55 (1994)

[6] A. Musesti, G.G.Giusteri, A. Marzocchi: Predicting Ageing: On the Mathematical Modelization of Ageing Muscle Tissue, in G. Riva et al. (Eds.), Active Ageing and Healthy Living, Chapter 17 (2014)

A Cahn - Hilliard type model with degenerate mobility and single-well potential. Convergence and error analysis of a finite element discretization.

Abramo Agosti
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
abramo.agosti@polimi.it

Paola Francesca Antonietti
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
paola.antonietti@polimi.it

Pasquale Ciarletta
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
pasquale.ciarletta@polimi.it

Maurizio Grasselli
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
maurizio.grasselli@polimi.it

Marco Verani
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
marco.verani@polimi.it

In this presentation we introduce a Cahn-Hilliard type equation with degenerate mobility and single-well potential of Lennard-Jones type, which models the evolution and growth of biological cells such as solid tumors. In this model the degeneracy set of the equation and the singularity set of the cellular potential do not coincide, and the absence of cells is an unstable equilibrium configuration of the potential. This features introduce a nontrivial difference with respect to the Cahn-Hilliard type equations analyzed in the literature so far. We formulate a finite element approximation of the problem, where the positivity of the solution is enforced by means of a discrete variational inequality. We prove the existence and uniqueness of the discrete solution, together with the convergence to the weak solution, and we study the error analysis of the approximation. We also present simulation results, by which we verify the a-priori error estimates and study the dynamics of the spinodal decomposition and the growth and scaling laws of phase ordering dynamics.

Small–scale Solid and Fluid Mechanics in Biology - Part II

PROPOSERS

Davide Ambrosi
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
davide.ambrosi@polimi.it

Paolo Zunino
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
paolo.zunino@polimi.it

SPEAKERS

Tobias Köppl
University of Stuttgart
tobias.koeppl@iws.uni-stuttgart.de

Timo Koch
University of Stuttgart
timo.koch@iws.uni-stuttgart.de

Raimondo Penta
Technische Universität Darmstadt
penta@mathematik.tu-darmstadt.de

Paolo Decuzzi
Istituto Italiano di Tecnologia
paolo.decuzzi@iit.it

Giuseppe Pascazio
Politecnico di Bari
giuseppe.pascazio@poliba.it

Alessandro Coclite
Istituto Italiano di Tecnologia
alessandro.coclite@iit.it

The minisymposium aims to gather the italian community of scientists working on the mathematical modelling and numerical simulation of mechanobiology at a tissue scale, with an emphasis on the biomedical perspective. Specific issues of interest will be the microcirculation, the growth of malignant tissues, the cellular and subcellular mechanics, nanomedicine and muscles. Both experimental, modeling and numerical methodologies will be tackled.

Numerical analysis of multi-dimensional models for network flow in biological systems

Tobias Köppl
University Stuttgart
Pfaffenwaldring 61, 70569 - Stuttgart Germany
tobias.koeppl@iws.uni-stuttgart.de

Ettore Vidotto
Technical University Munich
Boltzmannstraße 3, 85748 Garching
ettore.vidotto@ma.tum.de

Barbara Wohlmuth
Technical University Munich
Boltzmannstraße 3, 85748 Garching
barbara.wohlmuth@ma.tum.de

Paolo Zunino
Politecnico di MIlano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
paolo.zunino@polimi.it

Network structures can be detected in almost every biological system, since they are often responsible for the transport of fluids, nutrients or oxygen [1]. Such a network structure is for example a blood vessel network supplying organs with oxygenated blood or removing metabolic waste from the tissue [2]. A further example is the root network of a plant, ensuring the water supply of the plant [3] (see Figure 1). One way to obtain a

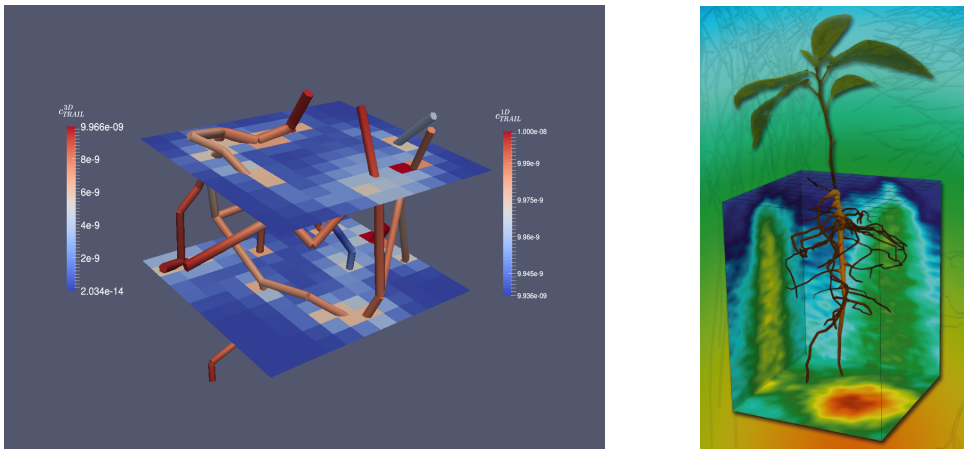


Figure 1: Mass transport in a capillary network embedded in tumor tissue (left), root network supplying a plant (right).

realistic model for such processes is based on a domain decomposition approach. Thereby,

the network structure is separated from the surrounding medium and different models are assigned to both domains. Quite often the surrounding medium (e.g. tissue or soil) can be considered as a three-dimensional (3D) porous medium. In order to decrease computational costs while maintaining a certain degree of accuracy, flow and transport processes within the networks are modeled by one-dimensional (1D) PDE-systems. A coupling of the network and the porous medium model is achieved by first averaging the 3D quantities and projecting them onto the 1D network structure. As a next step, the difference of the averaged 3D and 1D quantities is computed and incorporated into the source terms of both the network and the porous medium model, where the source term of the 3D problem exhibits a Dirac measure concentrated on the 1D network [4, 6].

In this talk we are concerned with the numerical analysis of PDE systems arising in the context of this model concept [5, 7]. In particular, it is investigated how the Dirac source terms and averaging operators affect the convergence behavior of standard finite element methods. Therefore, elliptic and parabolic model problems with Dirac source terms and averaging operators are investigated. Our theoretical results are confirmed by numerical tests.

References

[1] Köppl, Tobias and Wohlmuth, Barbara and Helmig, Rainer, 2013, *Reduced one-dimensional modelling and numerical simulation for mass transport in fluids*. International Journal for Numerical Methods in Fluids 72(2), 135–156.

[2] Cattaneo, Laura and Zunino, Paolo, 2014, *Computational models for fluid exchange between microcirculation and tissue interstitium*. Networks & Heterogeneous Media 9(1).

[3] Schröder, Natalie and Javaux, Mathieu and Vanderborght, Jan and Steffen, Bernhard and Vereecken, Harry, 2012, *Effect of root water and solute uptake on apparent soil dispersivity: a simulation study*. Vadose Zone Journal 11(3).

[4] D'Angelo, Carlo and Quarteroni, Alfio, 2008, *On the coupling of 1d and 3d diffusion-reaction equations: Application to tissue perfusion problems*. Mathematical Models and Methods in Applied Sciences, 18(8), 1481–1504.

[5] D'Angelo, Carlo, 2012, *Finite element approximation of elliptic problems with Dirac measure terms in weighted spaces: applications to one-and three-dimensional coupled problems*. SIAM Journal on Numerical Analysis, 50(1), 194–215.

[6] D'Angelo, Carlo, 2007, *Multi scale modelling of metabolism and transport phenomena in living tissues, PhD Thesis*. EPFL, Lausanne.

[7] Köppl, Tobias and Wohlmuth, Barbara, 2014, *Optimal a priori error estimates for an elliptic problem with Dirac right-hand side*. SINUM, 52(4), 1753-1769.

Modeling root water uptake and vascularized biological tissue using embedded multi-dimension methods with finite volumes

Timo Koch
University of Stuttgart, IWS/LH2
Pfaffenwaldring 61, 70569 - Stuttgart Germany
timo.koch@iws.uni-stuttgart.de

Katharina Heck
University of Stuttgart, IWS/LH2
Pfaffenwaldring 61, 70569 - Stuttgart Germany
katharina.heck@iws.uni-stuttgart.de

Bernd Flemisch
University of Stuttgart, IWS/LH2
Pfaffenwaldring 61, 70569 - Stuttgart Germany
bernd.flemisch@iws.uni-stuttgart.de

Rainer Helmig
University of Stuttgart, IWS/LH2
Pfaffenwaldring 61, 70569 - Stuttgart Germany
rainer.helmig@iws.uni-stuttgart.de

Mathematical models of flow and transport processes in and between the microcirculation and the surrounding tissue can contribute to understanding complex biological processes and guide treatment of vascular diseases and cancer. Models of root water uptake, nutrient uptake in crops and soil evaporation processes can help to make crop cultivation more efficient and to understand plant behavior in drying soils. The vast number of vessels, i.e. roots or blood capillaries, demand dimensionally reduced models of the network systems to describe the interaction with the surrounding bulk domain on a reasonable scale. Both problem can be tackled by the recently introduced embedded multi-dimension methods.

Embedded multi-dimension methods or embedded multi-scale methods with a dimensional gap of two were firstly introduced and analyzed in a mathematical framework in [1]. However, very similar methods have been suggested earlier for the modeling of plant root water uptake in [2, 3]. The methods feature two coupled PDE systems, one posed on a three-dimensional bulk domain, the other posed on a one-dimensional network domain that is geometrically embedded in three-dimensional space. They present an improvement over methods where micro-scale quantities are volume-averaged and upscaled yielding homogenized model descriptions on the macro-scale. Instead of upscaling certain interesting features, as the capillary network in a vascularized biological tissue or the root system of plants, these features are discretely resolved.

We present a new idea how to derive those models motivated by the fluid processes and the geometrical embedding in the bulk domain and the included network feature. The coupling

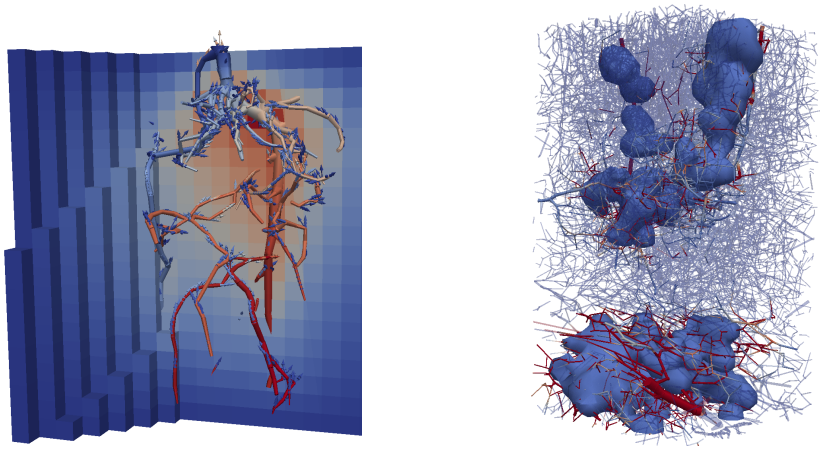


Figure 1: Left – pressure distribution in lupine root system and saturation in soil. Right – proliferation of a therapeutic agent through capillaries and tissue. Bubbles show mass-fraction isosurfaces in the tissue. Color visualizes mass fraction in the capillary network.

between the network domain and the volume-averaged bulk domain can be interpreted as numerical upscaling of the network domain. We compare the multi-dimension model with fully volume-averaged models on the same domain model-theoretically and numerically. We investigate the question of model limitation with respect to the grid resolution of the network and the bulk domains.
As application examples, we present an improved root water uptake model including soil evaporation processes to the atmosphere using an embedded multi-dimension method with finite volume discretization (see left figure). The independent grids allow for easy modification of the root architecture, and even for the modeling of root growth sensitive to soil parameters. As a second application we present the transport of a therapeutic agent TRAIL in tumorous tissue (see right figure). Studies on small vessel networks for drug profileration in tumorous tissue were conducted by [5]. Studies on larger networks by [4] used a dual continuum model description in a volume-averaged sense to be able to model larger domains. We suggest that an embedded multi-dimension method with finite volume discretization might be a solution to bridge the scales between micro and organ-scale.

References

[1] D'Angelo, C. 2007 *Multiscale Modelling of Metabolism and Transport Phenomena in Living Tissues*, PhD thesis, EPFL Lausanne.

[2] Doussan, C. and Pagès, L. and Vercambre, G. 1998 *Modelling of the hydraulic architecture of root systems: an integrated approach to water absorption—model description.* Annals of botany 81(2), 213–223.

[3] Javaux, M. and Schröder, T. and Vanderborght, J. and Vereecken, H. 2008 *Use of a Three-Dimensional Detailed Modeling Approach for Predicting Root Water Uptake.* Vadose Zone Journal 7(3), 1079ff.

[4] Erbertseder, K., Reichold, J., Flemisch, B., Jenny, P., Helmig, R. 2012 *A Coupled Discrete/Continuum Model for Describing Cancer-Therapeutic Transport in the Lung.* PLoS ONE 7(3).

[5] Cattaneo, L., Zunino, P. 2014 *A computational model of drug delivery through microcirculation to compare different tumor treatments*. Int. J. Numer. Meth. Biomed. Engng. 30(11) 1347–1371.

Can a continuous mineral foam explain the stiffening of aged bone tissue?

Raimondo Penta
Universidad Politecnica de Madrid, E.T.S. Ing. Caminos, Canales y Puertos
Calle del Prof. Aranguren, 3, 28040 Madrid, Spain.
penta@mathematik.tu-darmstadt.de

Kay Raum
Berlin-Brandenburg School for Regenerative Therapies, Charité Universitätsmedizin Berlin
Augustenburger Platz 1, 13353 Berlin, Germany

Quentin Grimal
Sorbonne Universités UPMC Univ Paris 06, CNRS, INSERM, Laboratoire d'Imagerie Biomedicale,
F-75006, Paris, France

Susanne Schrof
Berlin-Brandenburg School for Regenerative Therapies, Charité Universitätsmedizin Berlin
Augustenburger Platz 1, 13353 Berlin, Germany

Alf Gerisch
AG Numerik, FB Mathematik, TU Darmstadt
Dolivostr. 15, 64293, Darmstadt, Germany
gerisch@mathematik.tu-darmstadt.de

Recent experimental data revealed a stiffening of aged cortical bone tissue, which could not be explained by common multiscale elastic material models. We explain this data by incorporating the role of mineral fusion via a new hierarchical modeling approach exploiting the asymptotic (periodic) homogenization (AH) technique for three dimensional linear elastic composites. We quantify for the first time the stiffening that is obtained by considering a fused mineral structure in a softer matrix in comparison with a composite having non-fused cubic mineral inclusions. We integrate the AH approach in the Eshelby-based hierarchical mineralized turkey leg tendon model [1], which can be considered as a base for musculoskeletal mineralized tissue modeling. We model the finest scale compartments, i.e. the extrafibrillar space and the mineralized collagen fibril, by replacing the self-consistent scheme with our AH approach. This way, we perform a parametric analysis at increasing mineral volume fraction, by varying the amount of mineral that is fusing in the axial and transverse tissue directions in both compartments. Our effective stiffness results are in good agreement with those reported for aged human radius and support the argument that the axial stiffening in aged bone tissue is caused by the formation of a continuous mineral foam. Moreover, the proposed theoretical and computational approach supports the design of biomimetic materials which require an overall composite stiffening without increasing the amount of the reinforcing material.

References

[1] Tiburtius, S., Schrof, S., Molnár, F., Varga, P., Peyrin, F., Grimal, Q., ... and Gerisch, A. (2014). On the elastic properties of mineralized turkey leg tendon tissue: multiscale model and experiment. Biomechanics and modeling in mechanobiology, 13(5), 1003-1023.

Computational Nanomedicine: a world of opportunities for Computational Scientists and Applied Mathematicians

Paolo Decuzzi
Istituto Italiano di Tecnologia
via Morego 30, 16163 - Genova Italy
paolo.decuzzi@iit.it

The term "nanomedicine" is generally interpreted as the application, integration, and translation of nanotechnology to biomedical sciences. Nanomaterials with a characteristic size ranging between 1 and 100 nm manifest unique, size-dependent properties in physico-chemical phenomena and can be effectively used to manipulate, measure, stimulate, and perturb a biological system. Over the last decade, a myriad of devices and systems at the nanoscale have been developed for the diagnosis, imaging, and therapy of diseases. These include nanoparticles for the systemic delivery of imaging and therapeutic agents; nano/micro-fluidic systems for organ-on-a-chips; metallic nanoparticles for molecular sensing; electromagnetic nanosensors for the operation and control of medical devices; nanofibers for tissue engineering; and many others. The large majority of these nanosystems have been developed following a rather empirical approach, while the notion of rationally designing nanostructures, nanodevices, and nanoparticles has been only recently realized.
The use of computational modelling in the design of nanostructures and nanodevices for biomedical applications would certainly help in optimizing their performance in vivo and in understanding/predicting the detailed behavior of the biological system, per se. As such, the objective of this lecture is to emphasize the importance of "Computational Nanomedicine" as a critical tool for facilitating the integration of nanotechnology with biomedical sciences. As computational mechanics has already had a profound impact on science and technology over the last decades, we expect that Computational Nanomedicine could have an equally pervasive impact in rationally designing nanostructures, nanodevices, and nanoparticles for biomedical applications. The lecture will focus on three major topics: i) the rational design of non-spherical nanoconstructs for the systemic delivery of therapeutic and imaging agents; ii) the development of nanoparticles for more efficient Magnetic Resonance imaging; and iii) the analysis of tumor growth and metastatization in different biological environments [1, 2, 3, 4, 5].

References

[1] Ananta, Jeyarama S.; Godin, Biana; Sethi, Richa; et al. Geometrical confinement of gadolinium-based contrast agents in nanoporous particles enhances T-1 contrast *NATURE NANOTECHNOLOGY Volume: 5 Issue: 11 Pages: 815-821* Published: NOV 2010

[2] Decuzzi, P.; Godin, B.; Tanaka, T.; et al. Size and shape effects in the biodistribution of intravascularly injected particles *JOURNAL OF CONTROLLED RELEASE*

Volume: 141 Issue: 3 Special Issue: SI Pages: 320-327 Published: FEB 15 2010

[3] Decuzzi, Paolo; Pasqualini, Renata; Arap, Wadih; et al. Intravascular Delivery of Particulate Systems: Does Geometry Really Matter? *PHARMACEUTICAL RESEARCH Volume: 26 Issue: 1 Pages: 235-243* Published: JAN 2009

[4] Lee, Tae-Rin; Choi, Myunghwan; Kopacz, Adrian M.; et al. On the near-wall accumulation of injectable particles in the microcirculation: smaller is not better *SCIENTIFIC REPORTS Volume: 3 Article Number: 2079* Published: JUN 26 2013

[5] Sciume, G.; Shelton, S.; Gray, W. G.; et al. A multiphase model for three-dimensional tumor growth *NEW JOURNAL OF PHYSICS Volume: 15 Article Number: 015005* Published: JAN 16 2013

Margination dynamics of three-dimensional particles in shear flows

Giuseppe Pascazio
Politecnico di Bari
via Re David 200, 70125 - Bari - Italy
giuseppe.pascazio@poliba.it

Sergio Ranaldo
Politecnico di Bari
via Re David 200, 70125 - Bari - Italy
sergio.ranaldo@poliba.it

Alessandro Coclite
Istituto Italiano di Tecnologia
Via Morego 30, 16163 - Genova - Italy
alessandro.coclite@iit.it

Paolo Decuzzi
Istituto Italiano di Tecnologia
Via Morego 30, 16163 - Genova - Italy
paolo.decuzzi@iit.it

Marco Donato de Tullio
Politecnico di Bari
via Re David 200, 70125 - Bari - Italy
marcodonato.detullio@poliba.it

Understanding the margination dynamics of particles transported in fluids is a crucial aspect in the treatment and early-detection of cancer, having a direct relation with the number of the injected particles that reach the target tissue. A particle trasported in a channel that laterally marginates toward the wall during its motion has an enhanced probability of an efficient binding to specific targeted sites. This is a complicated dynamical process, in which the fluid dynamics plays an important role, including rolling events that are critical to the search process of particles near target, and strongly depend on the particle geometry [1]. In order to study the near wall dynamics of particles transported by the flow, a coupled Eulerian-Lagrangian approach is presented. The flow field is solved by means of a Lattice Boltzmann (LB) method [2] on a fixed Eulerian mesh, relying on a suitable Immersed Boundary (IB) technique to take into account the presence of moving and deforming bodies [3], while the suspended cells/particles are treated as Lagrangian solid domains immersed in the Eulerian fluid mesh [4, 5]. Individual particles will be modeled as membranes enclosing an incompressible fluid, and discretized by means of an unstructured triangular mesh [5, 6]. A weakly coupled fluid-structures interaction is employed, imposing the no-slip boundary condition on the surface of the solids and, after evaluating the hydrodynamic forces on the moving bodies, solving the rigid-body dynamic

equations. Numerical simulations will be performed to study the particle margination dynamics varying particle-related parameters, namely shape (sherical, ellipsoidal – either prolate or oblate –, discoidal, biconcave, biconvex), size and density, as well as flow-related parameters, such as shear rate, Reynolds number (at low values) and ratio between the channel height and particle main length. The main objective will be the evaluation of the effective lateral migration coefficient for the transported particles along with its rotation rate and equilibrium orientation with respect to the channel walls.

References

[1] G. Adriani, M.D. de Tullio, M. Ferrari, F. Hussain, G. Pascazio, X. Liu, and P. Decuzzi, 2012 *The preferential targeting of the diseased microvasculature by disk-like particles*. Biomaterials 33, 5504-5513.

[2] A. Coclite, G. Gonnella, and A. Lamura, 2014 *Pattern formation in liquid-vapor systems under periodic potential and shear*. Phys. Rev. E 89, 063303.

[3] M.D. de Tullio, A. Cristallo, E. Balaras, and R. Verzicco, 2009 *Direct numerical simulation of the pulsatile flow through an aortic bileaflet mechanical heart valve*. J. Fluid Mech. 622, 259-290.

[4] M. Vanella E. Balaras, 2009 *A moving-least-squares reconstruction for ebmedded-boundary formulations*. J. Comput. Phys. 228, 6617-6628.

[5] A. Coclite, M.D. de Tullio, G. Pascazio, and P. Decuzzi, 2016 *A combined Lattice Boltzmann and Immersed Boundary approach for predicting the vascular transport of differently shaped particles*. Comput. Fluids, under review.

[6] M.D. de Tullio, G. Pascazio, and M. Napolitano, 2012 Arbitrarily shaped particles in shear flow. In *Seventh International Conference on Computational Fluid Dynamics (ICCFD7)* 1303.

Vascular transport and adhesion mechanics of elliptical particle in capillary flows

Alessandro Coclite
Istituto Italiano di Tecnologia
Via Morego, 30 16163–Genova Italy
alessandro.coclite@iit.it

Marco Donato de Tullio
Politecnico di Bari
Via Re David, 200, 70125–Bari Italy
marcodonato.detullio@poliba.it

Giuseppe Pascazio
Politecnico di Bari
Via Re David, 200, 70125–Bari Italy
giuseppe.pascazio@poliba.it

Paolo Decuzzi
Istituto Italiano di Tecnologia
Via Morego, 30 16163–Genova Italy
paolo.decuzzi@iit.it

Modelling the vascular transport and adhesion of man-made particles is crucial for optimizing their biomedical efficacy as carriers of therapeutic and imaging agents [1, 2, 3]. Here, a Lattice Boltzmann (LB) and Immersed Boundary (IB) methods are combined together for predicting the dynamics of particles with different size and shapes in a laminar flow. For the LB modelling, the lattice equation is derived using a Gauss-Hermite projection [4], wall boundary conditions are imposed through the Zou-He framework [5], and a moving least square algorithm is used to accurately reconstruct the forcing term accounting for the presence of the immersed boundary [6]. The dynamics of particles immersed in the flow is simulated through a rigid-body–dynamics equations solver [7] weakly coupled iteratively with the flow solver.
First, mechanisms regulating the lateral drifting of particles across the stream lines, particle margination, are investigated as a function of the size, shape, and local hydrodynamic conditions. More specifically, elliptical particles with different aspect ratios, namely AR = 1 (i.e.: circles), 2 and 5 are considered with Reynolds number varying within a broad range (Re=0.001–5) representing small, medium, and large blood vessels of the circulatory system. Moreover, the ratio between the particle characteristic size and the vessel wall diameter, blockage ratio, is changed between 0.1 and 0.9.
Then, the particle surface is decorated with a uniform distribution of adhesive molecules, ligands, mediating the specific adhesive interaction with counter-molecules, receptors, distributed over the vessel walls. The molecular adhesive forces arising at the interface between the particle and the vessel wall is computed through a probabilistic approach determining bond formation and destruction over the entire particle surface [8]. Therefore,

the specific vascular adhesion can be estimated as a function of different hydrodynamic conditions and of the particle size, shape, and surface coating. While aspect ratios, blockage ratios and Reynolds number vary within the ranges defined above, four different surface densities of ligand molecules are considered providing a 30, 50, 70, and 90% coverage of the total particle surface. In conclusion, this work presents a computational model for predicting the vascular dynamics of particles in terms of their geometrical and biophysical properties within blood vessels of different calibre. This model would support the rational design of more efficient nanomedicines for theranosis in cancer, cardiovascular, and neurodegenerative diseases.

References

[1] G. Bao, Y. Bazilevs, J.-H. Chung, P. Decuzzi, H. Espinosa, M. Ferrari, H. Gao, S. Hossain, T. Hughes, R. Kamm, W. Liu, A. Marsden, B. Schrefler, Usnctam perspectives on mechanics in medicine, Journal of the Royal Society Interface 11 (97). doi:10.1098/rsif.2014.0301.

[2] S.-Y. Lee, M. Ferrari, P. Decuzzi, Shaping nano-/micro-particles for enhanced vascular interaction in laminar flows, Nanotechnology 20 (49) (2009) 495101.

[3] T.-R. Lee, M. Choi, A. M. Kopacz, S.-H. Yun, W. K. Liu, P. Decuzzi, On the near-wall accumulation of injectable particles in the microcirculation: smaller is not better, Scientific reports 3.

[4] A. Coclite, G. Gonnella, A. Lamura, Pattern formation in liquid-vapor systems under periodic potential and shear, Phys. Rev. E 89 (2014) 063303. doi:10.1103/PhysRevE.89.063303.

[5] Q. Zou, X. He, On pressure and velocity boundary conditions for the lattice boltzmann bgk model, Physics of Fluids 9 (6) (1997) 1591–1598. doi:http://dx.doi.org/10.1063/1.869307.

[6] M. Vanella, E. Balaras, A moving-least-squares reconstruction for embedded-boundary formulations, Journal of Computational Physics 228 (18) (2009) 6617 – 6628. doi:http://dx.doi.org/10.1016/j.jcp.2009.06.003.

[7] M. de Tullio, G. Pascazio, M. Napolitano, Arbitrarily shaped particles in shear flow, ICCFD7 proceedings (1303).

[8] C. Sun, C. Migliorini, L. L. Munn, Red blood cells initiate leukocyte rolling in postcapillary expansions: a lattice boltzmann analysis, Biophysical Journal 85 (1) (2003) 208–222.

Geometrically Unfitted Finite Element Methods

PROPOSERS

Anna Scotti
Politecnico di Milano
Pzza Leonardo da Vinci 32, 20133 - Milano Italy
anna.scotti@polimi.it

Sara Zahedi
KTH Royal Institute of Technology
100 44 Stockholm, Sweden
sara.zahedi@math.kth.se

Paolo Zunino
Politecnico di Milano
Pzza Leonardo da Vinci, 32 20133 - Milano Italy
paolo.zunino@polimi.it

SPEAKERS

Sara Zahedi (keynote)
KTH Royal Institute of Technology
sara.zahedi@math.kth.se

André Massing
Umea University
andre.massing@umu.se

Stefano Scialò
Politecnico di Torino
stefano.scialo@polito.it

Giulio Ventura
Politecnico di Torino
giulio.ventura@polito.it

Geometrically unfitted Finite Element Methods is a class of discretization methods for partial differential equations (PDEs) where the geometry is allowed to cut through the fixed background mesh on which the PDE is discretized. Boundary and interface conditions are usually imposed via a weak coupling and in many cases stabilization terms are added to handle cut elements. This technique allows for great flexibility in handling problems with heterogeneities and (moving) interfaces that can be non conforming with the computational grid, allowing for simple domain discretizations even in realistic applications with complicated and/or evolving geometries. This minisymposium aims at gathering researchers active on all aspects of these methods, including analysis, applications and implementation.

Space-Time Cut Finite Element Methods

Sara Zahedi
Department of Mathematics, KTH Royal Institute of Technology
SE-100 44 Stockholm, Sweden
sara.zahedi@math.kth.se

Peter Hansbo
Department of Mechanical Engineering, Jönköping University
SE-551 11 Jönköping, Sweden
peter.hansbo@ju.se

Mats G. Larson
Department of Mathematics and Mathematical Statistics, Umeå University
SE–901 87 Umeå, Sweden
mats.larson@math.umu.se

Finite element methods are famous for efficiently solving PDEs in complex geometries. However, when the geometry is moving the required remeshing and interpolation [3] leads to significant complications when the geometry undergoes strong deformations, especially in three space dimensions. We present a new computational method for solving Partial Differential Equations (PDEs) in dynamic geometries. Such PDEs occur in multiphase flow problems modeling for example the evolution of surfactants.
The model we consider is given by a time-dependent convection-diffusion equation on the interface separating two immiscible fluids coupled with a time-dependent convection-diffusion equation in the bulk. Our method [4] is based on a space-time formulation using discontinuous elements in time and continuous elements in space on a fixed background mesh. The interface can be arbitrarily located with respect to the background mesh and a cut finite element method is used to discretize the bulk and interface problems. In the cut finite element method the bilinear forms associated with the weak formulation of the problem are directly evaluated on the bulk domain and the interface, essentially using the restrictions of the basis functions to the computational domain. We add a consistent stabilization term [1] which ensures that 1) our method leads to linear systems with bounded condition number, 2) the numerical scheme for the surface PDE is stable also for convection dominated problems. In addition, the proposed method is very simple to implement since it only relies on spatial discretizations of the geometry at quadrature points in time and results in the same computations as in the case of stationary problems. Numerical results indicate that the method is optimal order accurate; we have also proven optimal order of accuracy for a related stationary coupled bulk-surface problem with a linear coupling term in [2].

References

[1] Burman, E. 2010 *Ghost penalty.* C. R. Acad. Sci. Paris, Ser. I 348 (21-22), 1217–1220.

[2] Burman, E., Hansbo, P., Larson, M. G., Zahedi. S. 2016, *Cut finite element methods for coupled bulk-surface problems*. Numer. Math. (in press). http://dx.doi.org/10.1007/s00211-015-0744-3

[3] Ganesan S. and Tobiska L. 2012, *Arbitrary Lagrangian–Eulerian finite-element method for computation of two-phase flows with soluble surfactants*. J. Comput. Phys. 231(9), 3685–3702.

[4] Hansbo, P., Larson, M. G., Zahedi. S. 2016, *A cut finite element method for coupled bulk-surface problems on time-dependent domains*. Comput. Methods Appl. Mech. Engrg. 307, 96–116.

A Discontinuous Cut Finite Element Framework for Multidimensional Multiphysics Problems

André Massing
Umeå University
90187 Umeå, Sweden
andre.massing@umu.se

Erik Burman
University College London
London, WC1E 6BT, United Kingdom
e.burman@ucl.ac.uk

Peter Hansbo
Jönköping University
55111 Jönköping, Sweden
peter.hansbo@ju.se

Mats G. Larson
Umeå University
90187 Umeå, Sweden
mats.larson@umu.se

We consider a discontinuous cut finite element framework for the numerical solution of PDEs posed on and and coupled through domains of different topological dimensionality. To allow for a flexible discretization and easy coupling with PDEs on lower dimensional manifold-type domains, the lower-dimensional geometries are embedded in an unfitted manner into a three dimensional background mesh consisting of tetrahedra. Since the embedded geometry is not aligned with the background mesh, we use the trace of discontinuous finite element functions defined on the tetrahedra as trial and test functions in the discrete variational formulations. As the resulting linear system may be severely ill-conditioned due to possibly small intersections between the embedded manifold and the background mesh, we discuss several possibilities for adding weakly consistent stabilizations terms to the original bilinear form. The proposed discretization schemes have optimal convergence properties and give raise to discrete linear systems which are well-conditioned independent of the intersection configuration. We conclude the presentation by illustrating the theoretical findings by a series of numerical experiments. As application examples, we consider a convection-diffusion interface-bulk problem with high constrast in the bulk diffusivity and the flow in porous media with fractures/faults.

References

[1] Burman, E., Claus, S., Hansbo, P., Larson, M., and Massing, A. CutFEM: discretizing geometry and partial differential equations. *Internat. J. Numer. Meth. Engng*, 104(7):472-501, November 2015.

[2] Burman, E., Hansbo, P., Larson, M., and Massing, A. A cut discontinuous Galerkin method for the Laplace-Beltrami operator. *IMA J. Numer. Anal.*, 2016.

[3] E. Burman, P. Hansbo, M. G. Larson, and A. Massing. Cut finite element methods for partial differential equations on embedded submanifolds of arbitrary codimension. *Submitted for publication.*, 2016b.

[4] D'Angelo, Carlo and Scotti, Anna (2012) A mixed finite element method for Darcy flow in fractured porous media with non-matching grids. *ESAIM: Mathematical Modelling and Numerical Analysis* **46(2)**, 465–489

Flow and transport simulations in fractured media with non-conforming meshes

Stefano Scialò
Politecnico di Torino
C.so Duca degli Abruzzi, 24, 10129 - Torino Italy
stefano.scialo@polito.it

Stefano Berrone
Politecnico di Torino
C.so Duca degli Abruzzi, 24, 10129 - Torino Italy
stefano.berrone@polito.it

Andrea Borio
Politecnico di Torino
C.so Duca degli Abruzzi, 24, 10129 - Torino Italy
andrea.borio@polito.it

Sandra Pieraccini
Politecnico di Torino
C.so Duca degli Abruzzi, 24, 10129 - Torino Italy
sandra.pieraccini@polito.it

Fabio Vicini
Politecnico di Torino
C.so Duca degli Abruzzi, 24, 10129 - Torino Italy
fabio.vicini@polito.it

Viable and effective simulations of the flow in underground reservoirs are a challenging task, of great importance for many practical applications such as the enhanced production of oil and gas, the geological disposal of pollutants or of nuclear waste, water resources management or geothermal applications. The subsoil is a porous medium characterized by the presence of discontinuities, such as inclusions or fractures. In some circumstances the fractures can significantly alter the flow properties and determine the preferential flow path such that the description of the fracture system is fundamental. Discrete Fracture Network (DFN) models can be used in this cases to provide a detailed description of the fractures in the subsoil that is thus modelled as a set of intersecting polygons, resembling the fractures in the underground, surrounded by a porous rock matrix.
The data for the generation of DFNs for a specific geological site are derived from on-site measurements and laboratory tests, in order to build probability distributions for quantities as the size, the orientation, the density and the hydraulic properties of the fractures and of the surrounding porous matrix. Difficulties in flow simulations in DFNs come from the geometrical complexity and the size of such computational domains (see Figure 1, left). Intersections among fractures, also called traces, are represented by segments in the model, and constitute interfaces of non-smoothness for the solution, and

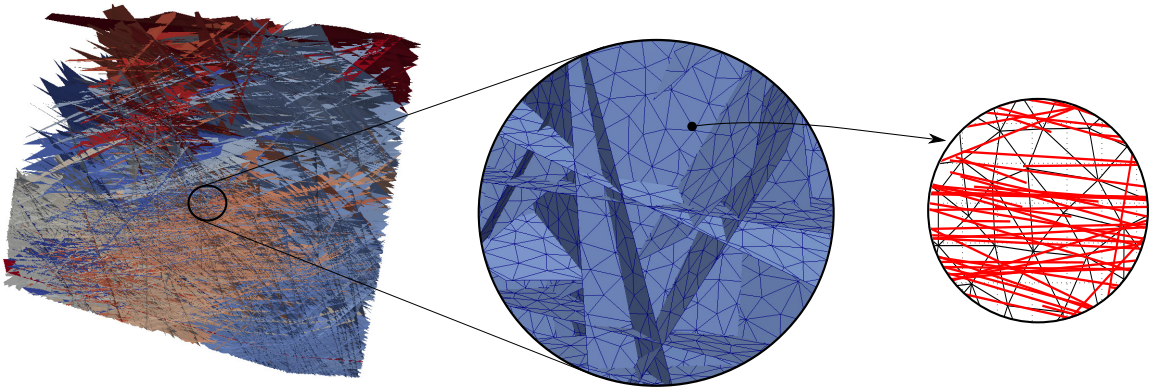


Figure 1: Example of a DFN and of a non-conforming mesh

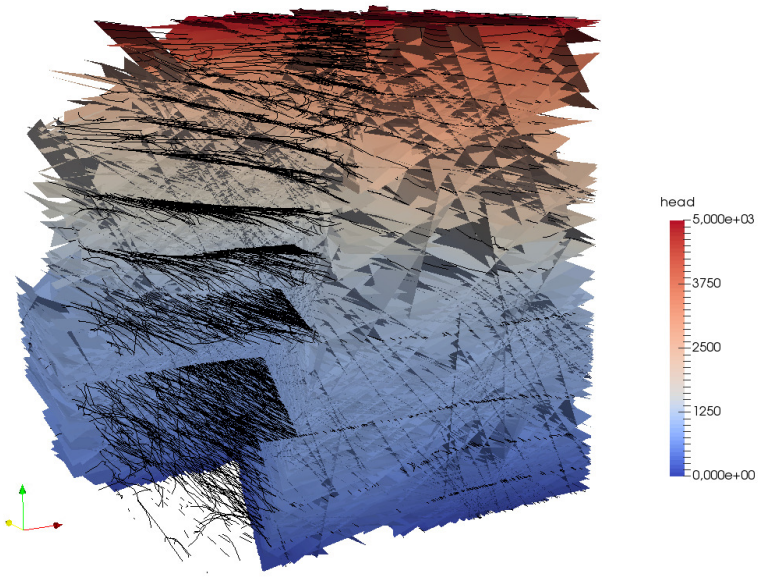


Figure 2: Stationary solution on a realistic network

problem-specific matching conditions need to be imposed at these interfaces. In realistic networks there can be a large number of traces in each fracture, intersecting each other with extremely narrow angles, or disposed very close to each other. Further, the traces in the same fracture can have lengths of different orders of magnitude, giving an intrinsic multi-scale nature to the problem.

Standard simulation approaches rely on meshes conforming at the intersections among fractures and on standard finite elements to compute the numerical solution. Conformity is needed in order to impose the matching conditions and to correctly reproduce the irregular behaviour of the solution at the traces. However, as a consequence of the mentioned geometrical issues, conforming meshes on DFNs are typically of low quality for the large number of geometrical constraints, or, in some cases, are even impossible to generate, for the same reason.

A new solution strategy has been recently proposed for the flow problem in DFNs,

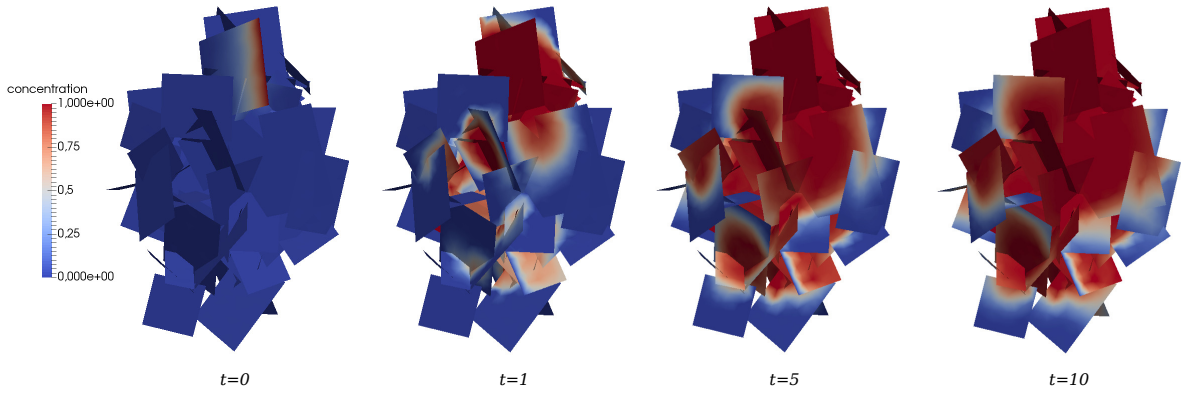


Figure 3: Four time-frames of a time-dependent simulation in a DFN

[4, 5, 6, 3, 2] that does not require mesh conformity at fracture intersections, as the mesh proposed in Figure 1. This approach is based on a PDE-constrained formulation of the problem, in which conditions at the interfaces correspond to the minimum of a properly designed cost functional. The solution of the problem is obtained minimizing this functional constrained by PDE equations in the interior of the fractures, expressing the governing law for the flow in the network. The structure of the cost functional can be devised in order to also prescribe boundary conditions to the problem [7], whereas the constraint equations can be customized to solve problems with different governing laws, as for example stationary/unsteady Darcy problems or unsteady advection-diffusion problems for the dispersion of pollutants [1]. The eXtended Finite Elment method (XFEM) [8] has been profitably combined with the method, in order to enhance the description of the solution near the traces on the non conforming meshes. Also, the optimization approach shows an intrinsically parallel nature that allows to efficiently tackle the size of the problem. The proven robustness of the method has been exploited for uncertainty quantification analyses bases on non intrusive approaches such as the stochastic collocation or multi-level Monte Carlo methods.

Numerical results have been provided on complex and realistic networks showing the viability and the performances of the proposed approach. The steady-state hydraulic-head problem was solved in large DFNs with highly heterogeneous hydraulic transmissivities, spanning several orders of magnitude, and with severe geometrical characteristics, see e.g. Figure 2. Solution quality is measured in terms of some error indicators also allowing for a comparison of the solution on networks with very different characteristics. Unsteady advection-diffusion problems describing the dispersion of pollutants in the underground have been solved, still in DFNs presenting all the geometrical complexities of realistic networks (see e.g. Figure 3). Advection-dominated flow regimes have been considered using stabilized approaches, thus providing a viable approach for time-dependent simulations in large and arbitrarily complex DFNs.

References

[1] S. Berrone, A. Borio, S. Pieraccini, and S. Scialò. Non-stationary transport phenomena in networks of fractures: effective simulations and stochastic analysis. Submitted for publication.

[2] S. Berrone, A. Borio, and S. Scialò. A posteriori error estimate for a PDE-constrained

optimization formulation for the flow in DFNs. *SIAM J. Numer. Anal.*, 54(1):242–261, 2016.

[3] S. Berrone, C. Canuto, S. Pieraccini, and S. Scialò. Uncertainty quantification in discrete fracture network models: stochastic fracture transmissivity. *Comput. Math. Appl.*, 70(4):603–623, 2015.

[4] S. Berrone, S. Pieraccini, and S. Scialò. A PDE-constrained optimization formulation for discrete fracture network flows. *SIAM J. Sci. Comput.*, 35(2):B487–B510, 2013.

[5] S. Berrone, S. Pieraccini, and S. Scialò. On simulations of discrete fracture network flows with an optimization-based extended finite element method. *SIAM J. Sci. Comput.*, 35(2):A908–A935, 2013.

[6] S. Berrone, S. Pieraccini, and S. Scialò. An optimization approach for large scale simulations of discrete fracture network flows. *J. Comput. Phys.*, 256:838–853, 2014.

[7] S. Berrone, S. Pieraccini, and S. Scialò. Towards effective flow simulations in realistic discrete fracture networks. *J. Comput. Phys.*, 310:181–201, 2016.

[8] Thomas-Peter Fries and Ted Belytschko. The extended/generalized finite element method: an overview of the method and its applications. *Internat. J. Numer. Methods Engrg.*, 84(3):253–304, 2010.

Quadrature and Stabilization of XFEM Formulations

Giulio Ventura
Politecnico di Torino
Corso Duca degli Abruzzi 24, 10129 - Torino Italy
giulio.ventura@polito.it

One of the most attractive properties of the eXtended Finite Element Method is its ability in dealing with discontinuities, interfaces and singularities without the need for the mesh to conform to these features. This is obtained by enriching the finite element approximation space by additional functions tailored to represent the physics of the particular problem at hand. Although the method is straightforward to implement and shows very good convergence properties, known shortcomings are how to effectively compute the enriched element matrices and how to deal with cases that may lead to indeterminate systems of equations, like in the case of a strong discontinuity crossing an element at a node.In this contribution a possible solution to these issues will be shown: quadrature based on equivalent polynomial mapping [1, 2] and enrichment independent penalty stabilization. The first allows to map Heaviside function enrichments on polynomials, allowing for a traditional Gaussian quadrature at the element level; the second introduces penalty stabilization terms for recovering a well conditions system of equations as well as a correction term to eliminate the unwanted effect of the penalty terms.

References

[1] Ventura, G. 2006 *On the elimination of quadrature subcells for discontinuous functions in the extended finite-element method.* Int. J. Numer. Meth. Engng. 66, 761–795.

[2] Ventura, G. and Benvenuti, E. 2015 *Equivalent polynomials for quadrature in heaviside function enriched elements.* Int. J. Numer. Meth. Engng. 102, 688–710.

Mean-field models in pedestrian dynamics

PROPOSERS

Marie-Therese Wolfram
Mathematics Institute, University of Warwick, CV4 7AL Coventry, UK
RICAM, Austrian Academy of Sciences, Altenbergerstr. 69, 4040 Linz, Austria
m.wolfram@warwick.ac.uk

SPEAKERS

Giacomo Albi
Technical University of Munich, Boltzmannstrasse 3, 85748 Garching
giacomo.albi@ma.tum.de

Elisabetta Carlini
Departimento di Matematica, Sapienza Universita di Roma, P.le Aldo Moro, 5, 00185 Rome
carlini@mat.uniroma1.it

Emiliano Cristiani
Istituto per le Applicazioni del Calcolo 'M Picone', Via dei Taurini 19, 00185 Rome
e.cristiani@iac.cnr.it

Adriano Festa
RICAM, Altenbergerstr. 69, 4040 Linz, Austria
adriano.festa@oeaw.ac.at

Paola Goatin
INRIA Sophia Antipolis, 06902 Sophia Antipolis Cedex, France
paola.goatin@inria.fr

Alessio Porretta
Universita di Roma Tor Vergata, Via della Ricerca Scientifica 1, 0133 Roma
porretta@mat.uniroma2.it

The complex dynamical behaviour of large pedestrian crowds has always fascinated researchers from various scientific fields. Academic studies began in earnest in the last century, starting with empirical observations in the early 1950's and continuing with the development of models in the field of applied physics. In recent years, applied mathematicians have become increasingly interested in analytical aspects as well as computational challenges related to simulation and calibration of pedestrian dynamics. The complex interactions between individuals as well as the physical surrounding result in non-linear partial differential equations or systems thereof, which often have a multi-scale nature.

This mini-symposium aims to highlight novel developments in the field of mean-field models for pedestrian dynamics. A special focus lies on the question how individual interactions and spatial structures such as networks lead to the organisation of pedestrian flows. We discuss recent analytic as well as computational findings for various nonlinear PDEs models as well as optimal control approaches.

Binary interaction approximation for mean-field optimal control problems

Giacomo Albi
Technische Univesität München
Boltzmannstr., 3, Garching bei München, Deutschland
giacomo.albi@ma.tum.de

In this talk I will present some recent developments on a class of numerical methods for the optimal control of multi-agent systems. Due to the high-dimensionality and the non-linearities of this type of problems, standard techniques usually fail or they are completely inefficient. In order to reduce the complexity of the problem, I will propose a general framework based on the approximation of the microscopic dynamics through a Boltzmann-like equation, showing that under a suitable scaling this is equivalent to the mean-field description of the original problem. Thereafter, I will present a set of algorithms, based on the simulation of the binary interactions of the Boltzmann dynamics, which allows to solve the mean-field optimal control problem. Several numerical example will show the efficiency of the proposed strategies in the context of crowd motion and opinion formations.

A Semi-Lagrangian scheme for a modified version of the Hughes model for pedestrian flow

Elisabetta Carlini
Sapienza Università d Roma
Piazzale A. Moro 2, 00185 - Rome Italy
carlini@mat.uniroma1.it

Adriano Festa
RICAM
Altenberger Straße 69, 4040 -Linz, Austria
adriano.festa@oaew.ac.at

Francisco J. Silva
Universitè de Limoges
33 rue François Mitterrand, 87032 Limoges - France
francisco.silva@unilim.fr

Marie-Therese Wolfram
University of Warwick and RICAM
Coventry CV4 7AL, UK
Altenberger Straße 69, 4040 -Linz, Austria
m.wolfram@warwick.ac.uk

We present a Semi-Lagrangian scheme for a regularized version of the Hughes model for pedestrian flow. In [3], R. Hughes proposed a macroscopic model for pedestrian dynamics, which is based on a continuity equation and an Eikonal equation, describing the evolution of a large pedestrian group trying to exit a domain as fast as possible. We consider this model in presence of small diffusion. The theoretical analysis of this regularized version of the Hughes model has been done in [2] in 1D with homogeneous Dirichlet boundary conditions.
We focus on the numerical analysis of the proposed Semi-Lagrangian scheme.
A Semi-Lagrangian scheme has been presented in [1] to deal with linear Fokker Plank equations. In this work, we propose an extension of the scheme in [1] in order to deal with nonlinear FP equations posed on a bounded domain and we use a Semi-Lagrangian scheme to numerically solve the stationary HJB equation. Furthermore we illustrate the effect of small diffusion on the exit time with various numerical experiments.

References

[1] Carlini E., Silva F. J. 2015 *A Semi-Lagrangian scheme for a degenerate second order mean field game system.* Discret Contin Dyn S 35(9):4269–4292.

[2] Di Francesco M, Markowich P A, Pietschmann F P, Wolfram M T 2011*On the Hughes' model for pedestrian flow: The one-dimensional case.* J Differ Equations 250(3):1334–1362.

[3] Hughes L. R. 2002 *A continuum theory for the flow of pedestrians.* Trasport Res B-Meth 36(6):507–535

Ill-posed mean-field games in pedestrian and vehicular traffic

Emiliano Cristiani
Istituto per le Applicazioni del Calcolo, CNR
e.cristiani@iac.cnr.it

Fabio S. Priuli
doge.fabio@gmail.com

Andrea Tosin
Politecnico di Torino
andrea.tosin@polito.it

In this talk we present a numerical investigation of two mean-field games which seem to be ill-posed, in the sense that multiple equilibria appear. The first model describes pedestrian flow in built environments [2], while the second one describes vehicular traffic on a road network [1]. Note that no second-order regularizing term is employed.
In both cases we face the problem of a large number of agents who aim at reaching a certain destination in minimal time. Agents are in competition since they move in the same domain and slow down each other with their presence. We assume agents to be perfectly rational, meaning that they are able to forecast with no errors the movements of the others at any time and decide their optimal path on the basis of their destination and the position of the others at both current and later times.
As a consequence, the models are constituted by a forward-backward system of PDEs. The first PDE is a conservation law which describes the evolution of the vehicle/pedestrian density given the optimal path from any origin to the desired destination. The second PDE is a Hamilton-Jacobi equation needed to solve the optimization problem which, in turn, depends on the whole distribution of agents in time and space. Preliminary numerical simulations show that multiple Nash equilibria of the systems exist. In particular, forward-backward iterations eventually oscillate between two possible solutions, without reaching convergence, cf. [3].

References

[1] Cristiani, E. and Priuli, F. S. 2015 *A destination-preserving model for simulating Wardrop equilibria in traffic flow on network*. Netw. Heterog. Media 10, 857–876.

[2] Cristiani, E., Priuli, F. S. and Tosin, A. 2015 *Modeling rationality to control self-organization of crowds: an environmental approach*. SIAM J. Appl. Math. 75, 605–629.

[3] Cacace, S., Cristiani, E., Falcone, M. 2013 *Numerical approximation of Nash equilibria for a class of non-cooperative differential games*. In: L. Petrosjan, V. Mazalov (eds.), Game Theory and Applications, Vol. 16, Chap. 4, 45–58, Nova Publishers, New York.

A discrete Hughes' model for pedestrian flow on graphs

Adriano Festa
RICAM - Austrian Academy of Sciences (ÖAW)
AltenbergerStrasse 4040 Linz, Austria
adriano.festa@oeaw.ac.at

Fabio Camilli
SBAI - Sapienza Universitá di Roma,
via Scarpa 16, 00161 Roma, Italy,
camilli@sbai.uniroma1.it

Silvia Tozza
Dip. di matematica - Sapienza Universitá di Roma,
P.le Aldo Moro 5, 00185 Roma, Italy.
tozza@mat.uniroma1.it

In this talk, we introduce a discrete time-finite state model for pedestrian flow on a graph in the spirit of the Hughes' dynamic continuum model [3, 1]. The pedestrians, represented by a density function, move on the graph choosing a route to minimize the instantaneous travel cost to the destination. The density is governed by a conservation law whereas the minimization principle is described by a graph eikonal equation (cf. [2]). We show that the discrete model is well-posed and the numerical examples reported confirm the validity of the proposed model and its applicability to describe real situations.

References

[1] E. Carlini, A. Festa, F.J. Silva and M.T. Wolfram, *A Semi-Lagrangian scheme for a modified version of the Hughes model for pedestrian flow* http://arxiv.org/abs/1601.07324

[2] F. Camilli, A. Festa and D. Schieborn, *An approximation scheme for a Hamilton-Jacobi equation defined on a network*, Appl. Numer. Math., **73** (2013), 33–47.

[3] R.L. Hughes, *A continuum theory for the flow of pedestrians*, Transport. Res. B-Meth., **36**(6) (2002), 507–535.

Non-local macroscopic models of traffic flow

Paola Goatin
Inria Sophia Antipolis Méditerranée
2004, route des Lucioles - BP 93, 06902 Sophia Antipolis Cedex, FRANCE
paola.goatin@inria.fr

Non-local interactions can be described through macroscopic models based on integro-differential equations. Systems of the form

$$\partial_t u + \mathrm{div}_{\mathbf{x}} F(t, \mathbf{x}, u, W) = 0, \qquad t > 0,\ \mathbf{x} \in \mathbb{R}^d,\ d \geq 1, \tag{1}$$

where $u = u(t, \mathbf{x}) \in \mathbb{R}^N$, $N \geq 1$ is the vector of the conserved quantities and the variable $W = W(t, x, u)$ depends on an integral evaluation of u, arise in a variety of physical applications. Space-integral terms are considered for example in models for granular flows [3], sedimentation [4], supply chains [10], conveyor belts [9] and biological applications like structured populations dynamics [11]. In particular, equations with non-local flux have been recently introduced in traffic flow modeling to account for the reaction of drivers or pedestrians to the surrounding density of other individuals, see [5, 6, 7, 12]. While pedestrians are likely to react to the presence of people all around them, drivers will mainly adapt their velocity to the downstream traffic, assigning a greater importance to closer vehicles. In particular, and in contrast to classical (without integral terms) macroscopic equations, these models are able to display finite acceleration of vehicles through Lipschitz bounds on the mean velocity [5] and lane formation in crossing pedestrian flows [1, 2]. We will also present recent results on micro-macro limits of empirical measures converging to measure-valued solutions of the corresponding macroscopic evolution equation [8].

References

[1] A. Aggarwal, R. M. Colombo, and P. Goatin. Nonlocal systems of conservation laws in several space dimensions. *SIAM J. Numer. Anal.*, 53(2):963–983, 2015.

[2] A. Aggarwal and P. Goatin. Crowd dynamics through non-local conservation laws. *Bulletin of the Brazilian Mathematical Society*, 47(1):37–50, 2016.

[3] D. Amadori and W. Shen. An integro-differential conservation law arising in a model of granular flow. *J. Hyperbolic Differ. Equ.*, 9(1):105–131, 2012.

[4] F. Betancourt, R. Bürger, K. H. Karlsen, and E. M. Tory. On nonlocal conservation laws modelling sedimentation. *Nonlinearity*, 24(3):855–885, 2011.

[5] S. Blandin and P. Goatin. Well-posedness of a conservation law with non-local flux arising in traffic flow modeling. *Numer. Math.*, 2015. Published online.

[6] J. A. Carrillo, S. Martin, and M.-T. Wolfram. A local version of the Hughes model for pedestrian flow. *Math. Models Methods Appl. Sci.*, 26(4):671–697, 2016

[7] R. M. Colombo, M. Garavello, and M. Lécureux-Mercier. A class of nonlocal models for pedestrian traffic. *Math. Models Methods Appl. Sci.*, 22(04):1150023, 2012.

[8] P. Goatin and F. Rossi. A traffic flow model with non-smooth metric interaction: well-posedness and micro-macro limit. *Commun. Math. Sci.*, to appear.

[9] S. Göttlich, S. Hoher, P. Schindler, V. Schleper, and A. Verl. Modeling, simulation and validation of material flow on conveyor belts. *Applied Mathematical Modelling*, 38(13):3295 – 3313, 2014.

[10] M. Gröschel, A. Keimer, G. Leugering, and Z. Wang. Regularity theory and adjoint-based optimality conditions for a nonlinear transport equation with nonlocal velocity. *SIAM J. Control Optim.*, 52(4):2141–2163, 2014.

[11] B. Perthame. *Transport equations in biology*. Frontiers in Mathematics. Birkhäuser Verlag, Basel, 2007.

[12] A. Sopasakis and M. A. Katsoulakis. Stochastic modeling and simulation of traffic flow: asymmetric single exclusion process with Arrhenius look-ahead dynamics. *SIAM J. Appl. Math.*, 66(3):921–944 (electronic), 2006.

Mean-field games modeling congestion effects in crowd dynamics

Alessio Porretta
Università degli Studi di Roma Tor Vergata
Via della Ricerca Scientifica 1, 00133 - Roma, Italy.
porretta@mat.uniroma2.it

A class of mean-field games models were introduced by J.M. Lasry and P.L. Lions to describe congestion and aversion effects in dynamics optimization within a population of many identical agents. The equilibria are solutions of forward-backward systems where Bellman and Fokker-Planck equations are strongly coupled and the Hamiltonian degenerates as the density of the agents becomes large. In this model the mean-field games system loses the variational character which is typical of a mean-field control formulation and some of the methods previously used cannot apply. In a joint work with Y. Achdou we prove existence and uniqueness results for this kind of mean-field games systems under general assumptions.

Advances in polygonal and polyhedral methods

PROPOSERS

Paola F. Antonietti
Politecnico di Milano
Pzza Leonardo da Vinci, 32 20133 - Milano Italy
paola.antonietti@polimi.it

Lourenco Beirao da Veiga
Università degli studi di Milano Bicocca
Via Cozzi 3, 20125 - Milano Italy
lourenco.beirao@unimib.it

Marco Verani
Politecnico di Milano
Pzza Leonardo da Vinci, 32 20133 - Milano Italy
marco.verani@polimi.it

SPEAKERS

Sandra Pieraccini (keynote)
Dipartimento di Scienze Matematiche, Politecnico di Torino
sandra.pieraccini@polito.it

Andrea Borio
Dipartimento di Scienze Matematiche, Politecnico di Torino
andrea.borio@polito.it

Lorenzo Mascotto
Dipartimento di Matematica, Università degli Studi di Milano
lorenzo.mascotto@unimi.it

Ilario Mazzieri
MOX-Dipartimento di Matematica, Politecnico di Milano
ilario.mazzieri@polimi.it

Giuseppe Vacca
Dipartimento di Matematica, Università degli studi di Bari
giuseppe.vacca@uniba.it

The interest in using general polytopes (as opposed to more standard tetrahedra and hexahedra) for the discretization of partial differential equations enjoyed a very large growth in recent years, with the blossoming of various new methods and further development of existing ones (to name a few: polygonal fem, gradient methods and finite volumes, virtual elements, mimetic finite differences, polygonal Discontinuous Galerkin, weak Galerkin methods). The community is growing large, and interaction among different standpoints becomes very important. The aim of this minisymposium is to discuss recent developments in this area. The proposed topics include (but are not limited to) recent advances on polyhedral methods with particular attention to challenges in code

development, fast solution techniques and application of polyhedral methods to real-life problems.

On the use of virtual element methods for underground flow simulations in fractured media

Sandra Pieraccini
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
sandra.pieraccini@polito.it

Matías Fernando Benedetto
Universidad de Buenos Aires
Buenos Aires - Argentina
matias.benedetto@polito.it

Stefano Berrone
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
stefano.berrone@polito.it

Andrea Borio
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
andrea.borio@polito.it

Stefano Scialò
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
stefano.scialo@polito.it

Subsurface flow simulation in a fractured medium is a challenging topic of great interest in several critical and up-to-date applications related to underground exploitation. Among these applications we mention geological storage, oil/gas enhanced production, water resources monitoring.
Among the possible approaches to underground fractured media modelization, we consider here the Discrete Fracture Network (DFN) approach. Within this model, the fractures crossing the rock matrix are modeled as planar polygons variously oriented in the space, thus forming a 3D set. We consider the rock matrix as impervious, and the flow occurs along fractures; flux exchange takes place across fracture intersections, which are called *traces*. An example of DFN is depicted in Figure 1.
The networks are typically generated starting from random distributions for geometrical features (such as orientation in the 3D space, position, dimension, and aspect ratio) and hydro-geological properties (transmissivity).
One of the major challenges in performing DFN flow simulations is given by the issue of generating good quality meshes on each fracture for computing the solution and imposing matching conditions between the solutions on different fractures.
Also due to the stochastic generation, such process should be robust, thus being effective

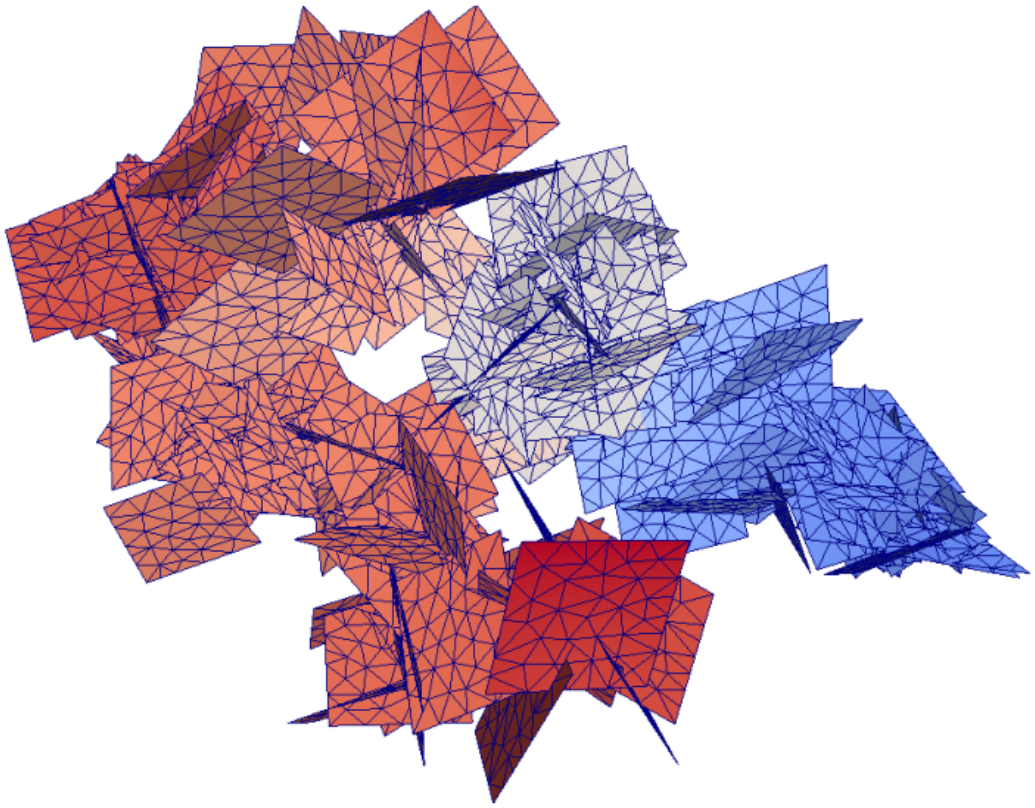


Figure 1: Example of DFN

on any arbitrary configuration, randomly generated. Namely, if classical triangular or quadrilateral meshes on the fractures are required to be conforming to the traces, and/or conforming each other, the meshing process for each fracture is fully dependent on the others. In this way, the mesh creation is a global process, yielding in practice a quite demanding computational effort. Furthermore, it may also result in an infeasible process, in some critical situations. In such cases some authors in recent literature prefer to modify the DFN removing problematic fractures. Here, we will discuss the application of the Virtual Element Method (VEM) [1] to the steady state simulation of the flow in DFNs. Within the approach proposed in recent works [3, 4, 5], we exploit the great deal of flexibility of VEM in using polygonal elements with an arbitrary number of edges, and also with parallel adjacent edges. This flexibility is used to efficiently tackle the geometrical complexity. More in details, in the approaches we are discussing herein, the VEM will be used within several possible solution techniques, which are coupled with several levels of mesh conformities: in conjunction with a PDE-constrained optimization approach [2, 3], with a totally non-conforming mesh; in conjunction with a mortar approach [4], introducing a partially conforming mesh; with a classical approach on a totally conforming polygonal mesh [5].

In all the approaches used, the VEM is exploited to tackle the interaction of mesh elements with the presence of traces. Indeed, we always start from a standard, arbitrary triangular mesh, independently built on each fracture, and independent of the trace disposition. Then, elements crossed by traces are cut in sub-elements. Trace tips falling inside an element, are prolonged up to the next element edge. With this procedure, elements with an arbitrary number of edges are obtained, possibly with vertices falling inside an edge, thus resulting in flat angles. An example of VEM mesh obtained with this procedure is

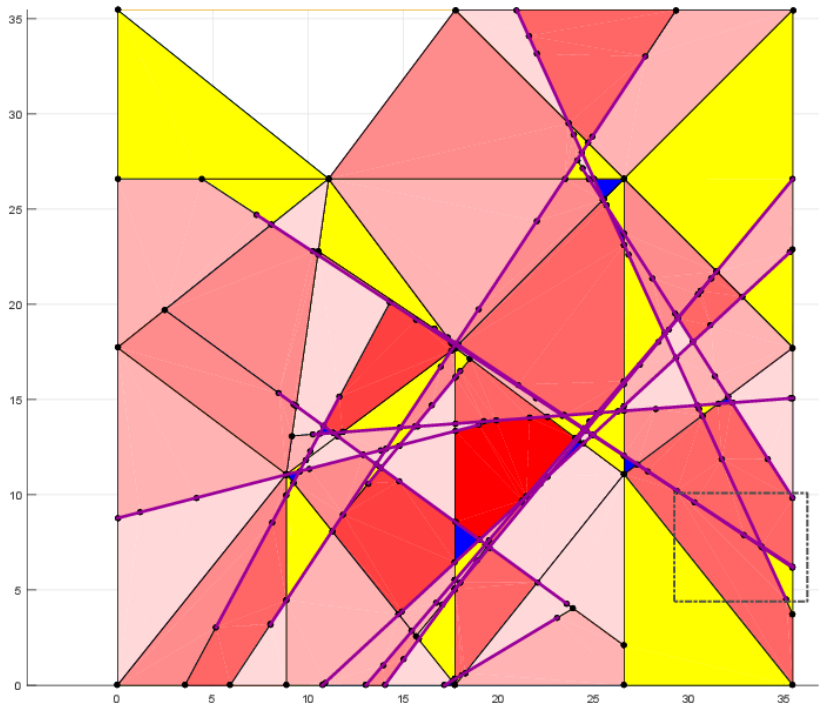


Figure 2: Example of polygonal mesh on a single fracture

depicted in Figure 2.

An optional mesh smoothing step can be performed, displacing element vertices, in such a way to improve the quality of the final polygonal mesh. Robustness and efficiency of the approach allow the application of the method to quite large and complex DFNs involving very complex geometrical situations like, for example, very small angles (less than one degree), coexistence of large and small fractures and both long and very short fracture intersections.

References

[1] Beirao da Veiga, L., Brezzi, F., Cangiani, A., Manzini, G., Marini, L. D. and Russo, A. 2013 *Basic Principles of Virtual Element Methods*. Mathematical Models and Methods in Applied Sciences 23, 199–214.

[2] Berrone, S., Pieraccini, S. and Scialò, S. 2014 *An optimization approach for large scale simulations of discrete fracture network flows*. Journal of Computational Physics 256, 838–853.

[3] Benedetto, F. M., Berrone, S., Pieraccini, S. and Scialò, S. 2014 *The Virtual Element Method for Discrete Fracture Network simulations*. Computer Methods in Applied Mechanics and Engineering 280, 135–156.

[4] Benedetto, F. M., Berrone, S., Borio, A., Pieraccini, S., and Scialò, S. 2016 *A Hybrid Mortar Virtual Element Method For Discrete Fracture Network Simulations*. J. Computational Physics 306, 148–166.

[5] Benedetto, F. M., Berrone, S. and Scialò, S. 2016 *A globally conforming method for solving flow in discrete fracture networks using the Virtual Element Method*. Finite Elements in Analysis and Design 109, 23–36.

A posteriori error estimates for the Virtual Element method in Discrete Fracture Network flow simulations

Andrea Borio
Politecnico di Torino
Corso Duca degli Abruzzi, 24, 10129 - Torino, Italy
andrea.borio@polito.it

Matías Fernando Benedetto
Politecnico di Torino
Corso Duca degli Abruzzi, 24, 10129 - Torino, Italy
matias.benedetto@polito.it

Stefano Berrone
Politecnico di Torino
Corso Duca degli Abruzzi, 24, 10129 - Torino, Italy
stefano.berrone@polito.it

Sandra Pieraccini
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
sandra.pieraccini@polito.it

Stefano Scialò
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
stefano.scialo@polito.it

Fabio Vicini
Politecnico di Torino
corso Duca degli Abruzzi, 24 10129 - Torino Italy
fabio.vicini@polito.it

The hydraulic head distribution inside a fractured medium can be computed, under suitable hypotheses, by modeling the medium with stochastically generated Discrete Fracture Networks (DFN, see Figure 1). Within this model the surrounding rock matrix is considered impervious and fractures are approximated by planar polygons mutually intersecting in space. The physical properties of the medium are suitably transformed in equivalent quantities that take the approximations into account. Using these models, uncertainty quantification strategies can be devised in order to compute quantities of interest such as mean value and variance for outgoing fluxes [9]. Those strategies require many repeated simulations, from which the need for efficient methods to solve pure diffusion or advection-diffusion problems. These numerical schemes should be able to deal with the many geometrical complexities that originate from the stochastic nature of

DFNs, generated by randomizing the orientation, dimension and aspect ratio of fractures. Among the resulting geometrical complexities, fracture sizes are usually very different, leading to problem in choosing a suitable meshsize to discretize the domain, and local meshes should be conforming to the intersections between fractures in order to be able to ensure continuity of the solution and balance of incoming and outcoming fluxes, while respecting the quality requirements that are requested to obtain an acceptable numerical solution.
In recent years, an interest is growing towards the development of numerical methods for PDEs designed to work on polythopal meshes. In this context, the Virtual Element Method (VEM) [1, 2] was developed, as an evolution of Mimetic Finite Difference Methods [3]. This new method allows the use of any kind of polygons (even featuring flat angles) to mesh the spatial domain and proves to be robust to bad quality elements. This flexibility is exploited in [6, 7, 5] to tackle the geometrical issues cited above by cutting an initial simplicial mesh at fracture intersections (see Figure 2), thus making possible to compute the hydraulic head distribution, that could then be used to obtain the Darcy velocity and simulate, for example, the transport of a passive scalar through the DFN. In this context, a VEM Streamline Upwind Petrov Galerkin formulation can be defined that preserves the rate of convergence of the method and cures the instabilities that arise when dealing with advection dominated problems [4]. Finally, the issue of estimating the error of approximation in a robust way with respect to jumps of the coefficient is of crucial importance to build adaptive strategies aiming at equidistributing the errors throughout the domain. A general framework can be established [8] to obtain a residual based a posteriori error estimator, depending on a suitably built polynomial projection of the discrete VEM solution and not on the stabilization form which is part of the VEM discrete formulation and is not fixed but only defined by its scaling properties. This estimator is robust with respect to jumps of the coefficients under certain standard hypotheses. This general framework can be applied with slight modifications to DFN simulations.

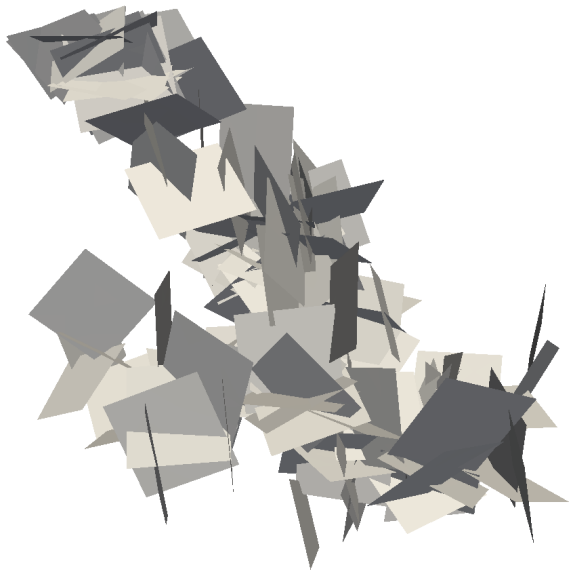


Figure 1: An example of Discrete Fracture Network.

References

[1] L. Beirão da Veiga, F. Brezzi, A. Cangiani, G. Manzini, L. D. Marini, and A. Russo. Basic principles of virtual element methods. *Mathematical Models and Methods in Applied Sciences*, 23(01):199–214, 2013.

[2] L. Beirão da Veiga, F. Brezzi, L. D. Marini, and A. Russo. Virtual element methods for general second order elliptic problems on polygonal meshes. *Mathematical Models and Methods in Applied Sciences*, 26(04):729–750, 2015.

[3] L. Beirão da Veiga, K. Lipnikov, and G. Manzini. *The Mimetic Finite Difference Method for Elliptic Problems*, volume 11 of *Modeling, Simulation & Applications*. Springer, 2014.

[4] M.F. Benedetto, S. Berrone, A. Borio, S. Pieraccini, and S. Scialò. Order preserving SUPG stabilization for the Virtual Element formulation of advection-diffusion problems. Submitted for pubblication.

[5] M.F. Benedetto, S. Berrone, A. Borio, S. Pieraccini, and S. Scialò. A hybrid mortar virtual element method for discrete fracture network simulations. *J. Comput. Phys.*, 306:148–166, 2016.

[6] M.F. Benedetto, S. Berrone, S. Pieraccini, and S. Scialò. The virtual element method for discrete fracture network simulations. *Comput. Methods Appl. Mech. Engrg.*, 280(0):135 – 156, 2014.

[7] M.F. Benedetto, S. Berrone, and S. Scialò. A globally conforming method for solving flow in discrete fracture networks using the virtual element method. *Finite Elem. Anal. Des.*, 109:23–36, 2016.

[8] S. Berrone and A. Borio. A residual a posteriori error estimate for the Virtual Element Method. In preparation.

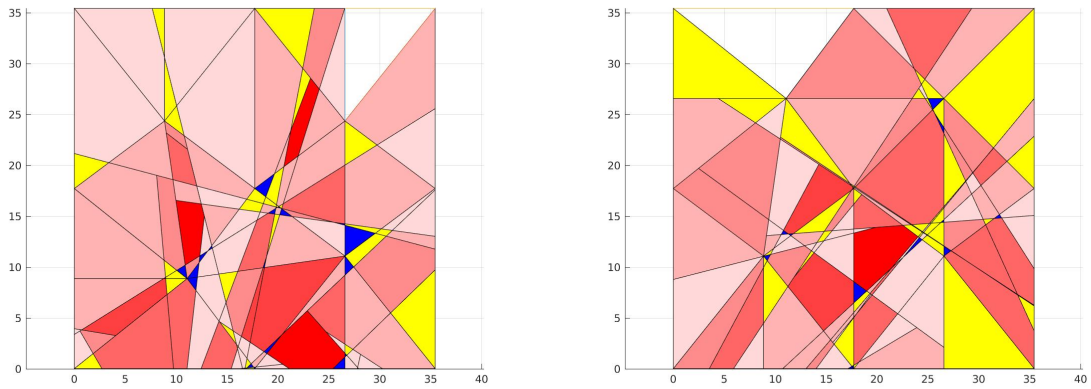


Figure 2: Examples of meshes used in the context of Virtual Element Methods applied to DFN simulations. Elements are colored depending on the number of sides.

[9] S. Berrone, C. Canuto, S. Pieraccini, and S. Scialò. Uncertainty quantification in discrete fracture network models: stochastic fracture transmissivity. *Comput. Math. Appl.*, 70(4):603–623, 2015.

The *hp* version of the virtual element method for corner singularities

Lorenzo Mascotto
Università degli Studi di Milano
via Saldini, 51 20133 - Milano Italy
lorenzo.mascotto@unimi.it

Lourenço Beirão da Veiga
Università degli Studi di Milano Bicocca
Via Cozzi, 55 20125 - Milano Italy
lourenco.beirao@unimib.it

Alexey Chernov
Carl von Ossietzky Universität
Ammerlander Heersträße, 114-118 G-26129 - Oldenburg Germany
alexey.chernov@uni-oldenburg.de

Alessandro Russo
Università degli Studi di Milano Bicocca
via Cozzi, 55 20125 - Milano Italy
alessandro.russo@unimib.it

The Virtual Element Method (VEM) is a recent generalization of the Finite Element Method (FEM), see [1]. The main features of VEM are the employment of polygonal/polyhedral meshes (thus including non conforming meshes) and the possibility of building easily global spaces of arbitrary regularity, see [4, 5].
In [2], the p version of VEM was introduced. p methods differ from their h counterparts since, while in the latter case the convergence of the error is achieved by mesh refinement, in the former the decomposition of the domain is kept fixed and the dimension of local spaces is increased. It was shown in [2] that, assuming high regularity of the solution, approximation by means of p VEM leads to exponential convergence of the energy error, while, whenever the solution has a *fixed* Sobolev regularity, the rate of convergence is only algebraic.
In the present talk, based on [3], after recalling the notation and the results of [2], we discuss about the approximation properties of VEM in presence of corner singularities, that is the approximation of functions analytic at the interior of the domain but with fixed Sobolev regularity at its corners. We also show that it is possible to prove exponential convergence of the errors in terms of the number of degrees of freedom.
VEM seems to be particularly appropriate for the numerical treatment of this kind of problems, since it allows for an automatic geometric refinement towards the corners of the domain, without the need of reshaping the mesh, as in FEM, in presence of hanging nodes. We also present a new stabilization of the method, on which explicit bounds on p are proven. Finally, numerical tests are shown.

References

[1] Beirão da Veiga, L. and Brezzi, F. and Cangiani, A. and Manzini, G. and Marini, L.D. and Russo, A. 2013 *Basic principles of Virtual Element Methods. Mathematical Models and Methods in Applied Sciences, 23(01), 199–214.*

[2] Beirão da Veiga, L. and Chernov, A. and Mascotto, L. and Russo, A. 2016 Basic principles of *hp* Virtual Elements on quasiuniform meshes. Mathematical Models and Methods in Applied Sciences, in press.

[3] Beirão da Veiga, L. and Chernov, A. and Mascotto, L. and Russo, A. Corner singularities and *hp* Virtual Elements, in preparations

[4] Beirão da Veiga, L. and Manzini, G. 2014 A virtual element method with arbitrary regularity. IMA Journal of Numerical Analysis, 34(2), 759–781.

[5] Brezzi, F. and Marini, L.D. 2012 Virtual Element Method for plate bending problems. Computer Methods in Applied Mechanics and Engineering 253, 455-462.

Discontinuous Galerkin methods for the elastodynamics problem on polygonal and polyhedral meshes

Ilario Mazzieri
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
ilario.mazzieri@polimi.it

Paola Francesca Antonietti
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
paola.antonietti@polimi.it

Antonio Nicolò
Politecnico di Milano
Piazza Leonardo da Vinci, 32 20133 - Milano Italy
antonio.nicolo@mail.polimi.it

In the field of computational seismology the use of advanced numerical methods has become a fundamental tool in the study of the complex phenomena arising in real geophysical applications. The physics governing these phenomena can be described through the use of the elastodynamics system. In the last years there has been an impressive progress worldwide towards the development of highly accurate numerical methods for the simulation of seismic wave propagation under realistic tectonic and geo-morphological conditions. The increasing need for flexible and certified numerical models apt to include the coupled effects of the seismic source, the propagation path through complex geological structures and localized superficial irregularities, such as alluvial basins or/and man-made infrastructures, still poses challenging demands on computational methods and resources due to the coexistence of very different spatial scales, from a few tens of kilometers, with reference to the seismic fault, up to a few meters, or even less, when considering some structural elements.

In this work we introduce a discontinuous Galekin (dG) finite element method (FEM) on meshes made of polygonal and polyhedral elements for the approximation of the elastodynamics equation in heterogeneous media. Under suitable assumptions, we prove the stability of the method and derive error estimates in a suitable mesh-dependent energy norm for the corresponding semidiscrete formulation. Moreover, we analyze the dissipation, dispersion and stability properties of the resulting scheme, when coupled with the Leap-Frog (LF) finite difference scheme. Numerical results for dGFEM on polytopic grids, are compared with those of the classical Spectral Element (SE) method on grids made by standard shaped elements. Finally, we apply the proposed method on benchmark as well as real test cases.

A stable Virtual Element Method for the Darcy equations and the Brinkman equations

Giuseppe Vacca
Università degli Studi di Bari
Via Edoardo Orabona, 4 70125 - Bari Italy
giuseppe.vacca@uniba.it

Lourenço Beirão da Veiga
Università degli Studi di Milano Bicocca
Via Cozzi, 55 20125 20133 - Milano Italy
lourenco.beirao@unimib.it

Carlo Lovadina
Università degli Studi di Pavia
Via Ferrata, 1 27100 - Pavia Italy
carlo.lovadina@unipv.it

The focus of the present talk is on developing a Virtual Element Method for the Darcy equations and for the Brinkman equations. In [6] we presented a family of Virtual Elements for the Stokes equations and we defined a new Virtual Element space of velocities such that the associated discrete kernel is pointwise divergence-free. We use a slightly different Virtual Element space for the Darcy equations having two fundamental properties: the L^2-projection onto $\mathbb{P}_k$ is exactly computable on the basis of the degrees of freedom, and the L^2 scalar product is coercive on the discrete kernel with coercivity constant h-independent instead of h^{-2} (if the discrete velocities in the kernel have vanishing divergence only in a projected sense as it happens for standard finite elements). The resulting numerical scheme has optimal order of convergence and continuous velocity solution. In particular we obtain a Virtual Element Method that is stable for both the Stokes and the Darcy equations. It is also natural to apply the same approach to the Brinkman equations than can be viewed as a combination of the Stokes and Darcy equations.

References

[1] L. Beirão da Veiga, F. Brezzi, A. Cangiani, G. Manzini, L. D. Marini, A. Russo. Basic principles of virtual element methods. Math. Models Methods Appl. Sci. 23 (2013), 199–214.

[2] B. Ahmad, A. Alsaedi, F. Brezzi, L. D. Marini, A. Russo. Equivalent projectors for virtual element methods. Comput. Math. Appl. 66 (2013), 376–391.

[3] L. Beirão da Veiga, F. Brezzi, L. D. Marini. Virtual elements for linear elasticity problems. SIAM J. Numer. Anal. 51(2) (2013), 794–812.

[4] L. Beirão da Veiga, F. Brezzi, L. D. Marini, A. Russo. Basic principles of mixed virtual element methods. ESAIM Math. Model. Numer. Anal. 48(4) (2014), 1227–1240.

[5] F. Brezzi, R. S. Falk, L. D. Marini. $H(\mathrm{div})$ and $H(\mathrm{curl})$-conforming VEM. Numer. Math. (2015), 1–30.

[6] L. Beirão da Veiga, C. Lovadina, G. Vacca. Divergence free virtual elements for the Stokes problem on polygonal meshes. In press in ESAIM: Mathematical Modelling and Numerical Analysis. arXiv preprint arXiv: 1510.01655 (2015).

[7] L. Beirão da Veiga, C. Lovadina, G. Vacca. A stable Virtual Element Method for the Darcy equations and the Brinkman equations. In preparation (2016).

Plenaries

High-order Discontinuous Galerkin methods for seismic wave propagation problems

Paola Antonietti
MOX, Dipartimento di Matematica
Politecnico di Milano

In this talk we present and analyse high order Discontinuous Galerkin methods for the space discretization of the elastodynamics equation. The proposed approach combines the flexibility of discontinuous Galerkin methods to connect together, through a domain decomposition paradigm, Spectral Element blocks where high-order polynomials are used. In such a way, the spatial discretisation and/or the local polynomial degree can be tailored to the region of interest.

This approach is particularly well suited for the simulation of complex wave phenomena, such as the seismic response of sedimentary basins or soil-structure interaction problems, where flexibility is crucial in order to simulate correctly the wave-front field. We analyse the semi-discrete formulation as well as the fully-discrete one, which is obtained through an explicit integration scheme. Some validation benchmarks are shown to verify the accuracy, stability and performance of the proposed approach.

We also present some simulations of real large-scale seismic events in three-dimensional complex media: from far-field to near-field including soil-structure interaction effects. The numerical results have been obtained with the high performance, open-source numerical code *SPEED* (see `https://speed.mox.polimi.it`).

Tools for spline-based methods

Annalisa Buffa
Istituto di Matematica Applicata e Tecnologie Informatiche del CNR
Pavia, Italy

In the last ten years the use of splines as a tool for the discretisation of partial differential equations has gained interests thanks to the advent of isogeometric analysis [1], [2]. In this context, the development of methods capable of alleviating the constraints on meshing imposed by the tensor product structure of spline spaces are needed and object of several studies. I will discuss a number of techniques going from mortaring approaches [4] to hierarchical splines for adaptivity [3]. For all methods I will discuss, I will present both theoretical and numerical results in the context of elliptic problems.

This research activity has been developed along the last years, in collaboration with several colleagues: C. Giannelli, B. Wolhmuth, L. Wunderlich, P. Antolin, F. Marini, M. Martinelli and G. Sangalli.

References

[1] T. J. R. Hughes, J. A. Cottrell, and Y. Bazilevs. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement. *Comput. Methods Appl. Mech. Engrg.*, 194 (2005), 4135–4195.

[2] J. A. Cottrell, T. J. R. Hughes, and Y. Bazilevs. *Isogeometric Analysis: toward integration of CAD and FEA*. John Wiley & Sons, 2009.

[3] A. Buffa, C. Giannelli. Adaptive isogeometric methods with hierarchical splines: error estimator and convergence. *Math. Models Methods Appl. Sci. 26 (2016), no. 1, 125.*

[4] E. Brivadis, A. Buffa, B. Wohlmuth, L. Wunderlich. Isogeometric mortar methods . *Comput. Methods Appl. Mech. Engrg. 284 (2015), 292319.*

Mathematical and numerical modeling for multiphysics problems

Alfio Quarteroni
CMCS, EPFL, Lausanne

When solving multiphysics problems, two basic issues need to be addressed: the mathematical formulation of the coupling mechanism that would be suitable for the numerical treatment and the efficient solution of the associated numerical problem that quite often features a very high dimension.

This presentation will touch upon both issues and will illustrate some recent ideas that have been elaborated for successfully coping with these challenges. In particular I will discuss the role of the Interface Control Domain Decomposition (*ICDD*) method to mathematically formulate the physical problem, the *INTERNODES* method for the numerical treatment of numerical non-conformities, and the *FaCSI* preconditioning strategy to efficiently solve the associated algebraic problem.

A few applications will be illustrated in the field of fluid dynamics, optimal design of parametrized problems , and life sciences.

Challenges in Computational and Data Science

Wil H.A. Schilders
Department of Mathematics and Computer Science
TU Eindhoven

For several decades, Computational Science has been recognized as the third discipline alongside the classical disciplines of theory and experimentation. Virtual design environments are commonplace by now, and used in all branches of industry. A prominent example is the virtual wind tunnel developed by the aerospace industry.

In recent years, a fourth discipline is emerging, centered around the availability of huge amounts of data, and therefore termed Data Science. Although the discipline so far appears to be claimed by computer scientists, there are many mathematical challenges, some naturally of a statistical nature but also in many other fields of mathematics. Especially interesting is the inter-linkage between computational and data sciences, also referred to as data driven science. The main aim remains to extract accurate models of phenomena and processes, but data driven science provides many more opportunities to address challenges that so far seemed unattainable, such as the 'tyranny of scales'. In this context, model order reduction is also rapidly becoming an indispensable tool.

In this presentation, we will discuss the general context, zoom in to a number of specific challenges and methodologies and give several examples.

Kinetic Models in Socio-Economic Sciences

Giuseppe Toscani
Department of Mathematics
University of Pavia

In recent years, the distribution of wealth in a multi-agent society has been investigated by resorting to classical methods of kinetic theory of rarefied gases [1]. In analogy with the Boltzmann equation, the change of wealth in these models is due to microscopic binary trades among agents. The same strategy has been recently applied to investigate new aspects linked to different types of human wealth, like the role of personal knowledge [2] (information), personal conviction [3] and others.

In this lecture, we introduce and discuss various nonlinear kinetic equations of Boltzmann type and related Fokker-Planck type equations which describe the evolution of these quantities. Also, the coupled evolution is dealt with.

As main example, we will study the influence of knowledge in the evolution of wealth in a system of agents which interact through binary trades. The trades, which include both saving propensity and the risks of the market, are here modified in the risk and saving parameters, which now are assumed to depend on the personal degree of knowledge.

The numerical simulations show that the presence of knowledge has the potential to produce a class of wealthy agents and to account for a larger proportion of wealth inequality.

References

[1] L. Pareschi, G. Toscani, *Interacting Multiagent Systems: Kinetic Equations and Monte Carlo Methods*, Oxford University Press, Oxford (2014)

[2] L. Pareschi, G. Toscani, Wealth distribution and collective knowledge. A Boltzmann approach, *Phil. Trans. R. Soc.* A 372, 20130396, 6 October (2014)

[3] C. Brugna, G. Toscani, Kinetic models of opinion formation in the presence of personal conviction, *Phys. Rev.* E 92, 052818 (2015)

Index of speakers

Index of authors

Index of plenary and keynote speakers