



bolla
lingotto

XX secolo

XIX secolo

mole
antonelliana

arco
olimpico

XXI secolo

porta
palatina

I secolo

palazzo
madama

I secolo - XVIII secolo

// TORINO 25-28 GIUGNO 2012

CONGRESSO NAZIONALE SIMAI

2012

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CONGRESSO
NAZIONALE SIMAI

2012

SIMAI 2012

Politecnico di Torino, June 25-28, 2012

The aim of **SIMAI Biannual Congresses** is to provide a scientific forum for presenting and discussing the issues and the advances in applied mathematics and applications of mathematics to industry, technology, environment, cultural heritage, biology and society.

By bringing together researchers and professionals in applied analysis, mathematical modeling and scientific computing, **SIMAI 2012** represents a key occasion to promote and stimulate interdisciplinary research in applied mathematics and to foster interactions with industry.

Conference Venue

Opening: (June 25, 2012)
Politecnico di Torino, Sala Consiglio di Facoltà
Corso Duca degli Abruzzi 24, 10129 Torino
Conference: (from June 25 to June 28, 2010)
Politecnico di Torino
Corso Duca degli Abruzzi 24, 10129 Torino

Invited Speakers

Luigi Barletti, Firenze
Paolo Bisegna, Roma
Antonio DeSimone, Trieste
Nicole El Karoui, Paris
Massimo Fornasier, München
Valeria Simoncini, Bologna

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Societa' Italiana di Matematica Applicata e Industriale
Via dei Taurini, 19 - 00185 Roma
www.simai.eu

Scientific Committee

Nicola Bellomo, Politecnico di Torino, *Chair*
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Luca Formaggia, Politecnico di Milano
Giorgio Fotia, CRS4 Bioinformatica, Pula (Cagliari)
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Anna Sciomachen, Università di Genova

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Luigi Preziosi, Politecnico di Torino
Luigia Puccio, Università di Messina

Graphic layout and cover design

TEMBO Communication Design, Torino

[SIMAI 2012]

ABSTRACTS

Updated on June 22, 2012

[SIMAI 2012]

Invited Speakers

Luigi Barletti, Università degli Studi di Firenze, Italy
Quantum fluid models for nanoelectronics

Paolo Bisegna, Università di Roma Tor Vergata, Italy
Mathematical issues in visual transduction

Antonio DeSimone, Scuola Internazionale Superiore di Studi Avanzati,
Trieste, Italy
Cellular motility: mechanical bases and some mathematical results

Nicole El Karoui, Ecole Polytechnique, Palaiseau, France
Dynamic utilities and long term interest rates

Massimo Fornasier, Technische Universität München, Germany
Random dimensionality reduction and sparse recovery algorithms

Valeria Simoncini, Università di Bologna, Italy
Solution of structured algebraic linear systems in PDE-constrained optimization problems

[SIMAI 2012]

Time table

Monday, June 25th

	ROOM	TIME
REGISTRATION	CdF	13:00 - 14:00
OPENING CEREMONY	CdF	14:00 - 14:30
PLENARY SESSION Nicole El Karoui Dynamic utilities and long term interest rates	CdF	14:30 - 15:30
COFFEE BREAK		15:30 - 16:00
PLENARY SESSION Valeria Simoncini Solution of structured algebraic linear systems in PDE-constrained optimization problems	CdF	16:00 - 17:00
WELCOME DRINK		19:00

Tuesday, June 26th

	ROOM	TIME
PARALLEL SESSIONS: MINISYMPOSIA		9:00 - 10:40
Approximation methods for data and image processing - I <i>Cotronei, Lamberti, Rossini</i>	4i	
Complex systems I <i>Sacerdote</i>	2i	
Integral equations: numerical methods and applications - I <i>Aimi, Diligenti, Monegato</i>	1i	
Mathematical problems in semiconductors and related topics - I <i>Muscato, Majorana, Romano</i>	5i	
New problems arising in mathematical modeling of smart and biological materials - I <i>Andreucci, Carillo</i>	3i	
Optimization methods for inverse problems in imaging and machine learning <i>Ruggiero, Zanni</i>	7i	
Variational inequalities and network equilibrium problems <i>Barbagallo, Maugeri</i>	6i	
COFFEE BREAK		10:40 - 11:10

[SIMAI 2012]

Time table

TIME	Tuesday, June 26th	ROOM
11:10 - 12:50	PARALLEL SESSIONS: MINISYMPOSIA Approximation methods for data and image processing - II <i>Cotronei, Lamberti, Rossini</i> Complex systems II <i>Sacerdote</i> Integral equations: numerical methods and applications - II <i>Aimi, Diligenti, Monegato</i> Mathematical and numerical modelling in geosciences <i>Miglio, Formaggia</i> Mathematical modelling in biomedicine I <i>Preziosi</i> Mathematical problems in semiconductors and related topics - II <i>Muscato, Majorana, Romano</i> New problems arising in mathematical modeling of smart and biological materials - II <i>Andreucci, Carillo</i>	4i 2i 1i 7i 6i 5i 3i
12:50 - 14:00	LUNCH BREAK	
12:50 - 14:00	LUNCH TIME SESSION HPC at CINECA: overview, new features and applications in Mathematics	1i
14:00 - 15:40	PARALLEL SESSIONS: MINISYMPOSIA Advances in numerical methods and applications I <i>Naldi</i> Complex systems III <i>Sacerdote</i> Developments of graph theory to networks - I <i>Imbesi, La Barbiera</i> Integral equations: numerical methods and applications - III <i>Aimi, Diligenti, Monegato</i> Mathematical problems in semiconductors and related topics - III <i>Muscato, Majorana, Romano</i> New problems arising in mathematical modeling of smart and biological materials - III <i>Andreucci, Carillo</i> Nonlinear evolution equations: analytical and geometrical methods - I <i>Demontis, Ortenzi</i>	7i 2i 4i 1i 5i 3i 6i

[SIMAI 2012]

Time table

Tuesday, June 26th

	ROOM	TIME
PARALLEL SESSIONS: MINISYMPOSIA		16:10 - 17:50
Advances in numerical methods and applications II <i>Naldi</i>	7i	
Developments of graph theory to networks - II <i>Imbesi, La Barbiera</i>	4i	
Integral equations: numerical methods and applications - IV <i>Aimi, Diligenti, Monegato</i>	1i	
Mathematical problems in semiconductors and related topics - IV <i>Muscato, Majorana, Romano</i>	5i	
New problems arising in mathematical modeling of smart and biological materials - IV <i>Andreucci, Carillo</i>	3i	
Nonlinear evolution equations: analytical and geometrical methods - II <i>Demontis, Ortenzi</i>	6i	
Topics in classical mechanics <i>Groppi</i>	2i	

Wednesday, June 27th

	ROOM	TIME
FOCUS SESSION		
Mathematics & Industry, a novel approach to R&D	1i	9:00 - 12:50
PARALLEL SESSIONS: MINISYMPOSIA		9:00 - 10:40
Computational and statistical methods for biomedical applications - I <i>Sangalli, Vergara</i>	6i	
Developments of graph theory to networks - III <i>Imbesi, La Barbiera</i>	4i	
From nano to macro: modeling and simulation <i>Riccardi</i>	7i	
Mathematical methods in decisions, economics, finance and games - I <i>Carfi, Ricciardello, Schilirò</i>	5i	
New problems arising in mathematical modeling of smart and biological materials - V <i>Andreucci, Carillo</i>	3i	

[SIMAI 2012]

Time table

TIME	Wednesday, June 27th	ROOM
	Reduced and polynomial approximation strategies for parametrized and stochastic PDEs - I <i>Tamellini, Manzoni</i>	2i
	Variational methods for problems in applied sciences - I <i>Chiadò Piat, Zappale</i>	8i
10:40 - 11:10	COFFEE BREAK	
11:10 - 12:50	PARALLEL SESSIONS: MINISYMPOSIA	
	Advances in numerical methods and applications III <i>Naldi</i>	7i
	Computational and statistical methods for biomedical applications - II <i>Sangalli, Vergara</i>	6i
	Mathematical methods in decisions, economics, finance and games - II <i>Carfi, Ricciardello, Schilirò</i>	5i
	Mathematical models for renewable energy sources <i>Felaco, Di Michele</i>	4i
	Networks and optimization <i>Chinnici</i>	2i
	Quasi-variational inequalities, generalized Nash equilibrium problems and applications <i>Scrimali</i>	3i
	Variational methods for problems in applied sciences - II <i>Chiadò Piat, Zappale</i>	8i
12:50 - 14:00	LUNCH BREAK	
14:00 - 15:00	PLENARY SESSION Luigi Barletti Quantum fluid models for nanoelectronics	CdF
15:00 - 16:00	PLENARY SESSION Massimo Fornasier (SIMAI Biannual Prize 2012 recipient) Random dimensionality reduction and sparse recovery algorithms	CdF
16:00 - 16:30	COFFEE BREAK	
16:30 - 18:00	ROUND TABLE ON MATHEMATICS AND INDUSTRY	CdF
20:00	SOCIAL DINNER	

[SIMAI 2012]

Time table

Thursday, June 28th

	ROOM	TIME
PARALLEL SESSIONS: MINISYMPOSIA		9:00 - 10:40
Beyond the mesh: handling geometry with unconventional methods <i>Scotti, Dassi</i>	7i	
Large-scale numerical linear algebra and optimization <i>Bellavia, De Simone</i>	2i	
Mathematical methods in decisions, economics, finance and games - III <i>Carfi, Ricciardello, Schilirò</i>	5i	
Mathematical modelling in biomedicine II <i>Preziosi</i>	6i	
Numerical modelling for engineering applications involving complex fluids and geometries - I <i>Berrone, Verani</i>	1i	
Packing optimization problems in space engineering <i>Fasano</i>	4i	
Topics in fluid dynamics I <i>De Bernardis</i>	3i	
COFFEE BREAK		10:40 - 11:10
PARALLEL SESSIONS: MINISYMPOSIA		11:10 - 12:50
Mathematical modelling in biomedicine III <i>Preziosi</i>	6i	
Numerical modelling for engineering applications involving complex fluids and geometries - II <i>Berrone, Verani</i>	1i	
Numerical resolution of PDE: the potentiality of the Life V library <i>Fumagalli, Dassi</i>	7i	
Reduced and polynomial approximation strategies for parametrized and stochastic PDEs - II <i>Tamellini, Manzoni</i>	2i	
Topics in fluid dynamics II <i>De Bernardis</i>	3i	
Topics in rational mechanics <i>Frosali</i>	4i	
LUNCH BREAK		12:50 - 14:00

[SIMAI 2012]

Time table

TIME	Thursday, June 28th	ROOM
14.00 - 15.00	PLENARY SESSION Antonio DeSimone Cellular motility: mechanical bases and some mathematical results	CdF
15.00 - 16.00	PLENARY SESSION Paolo Bisegna Mathematical issues in visual transduction	CdF
16.00 - 16.30	<i>COFFEE BREAK</i>	
16.30 - 17.30	ASSEMBLEA SOCI	CdF
17.30	<i>CLOSING CEREMONY</i>	CdF

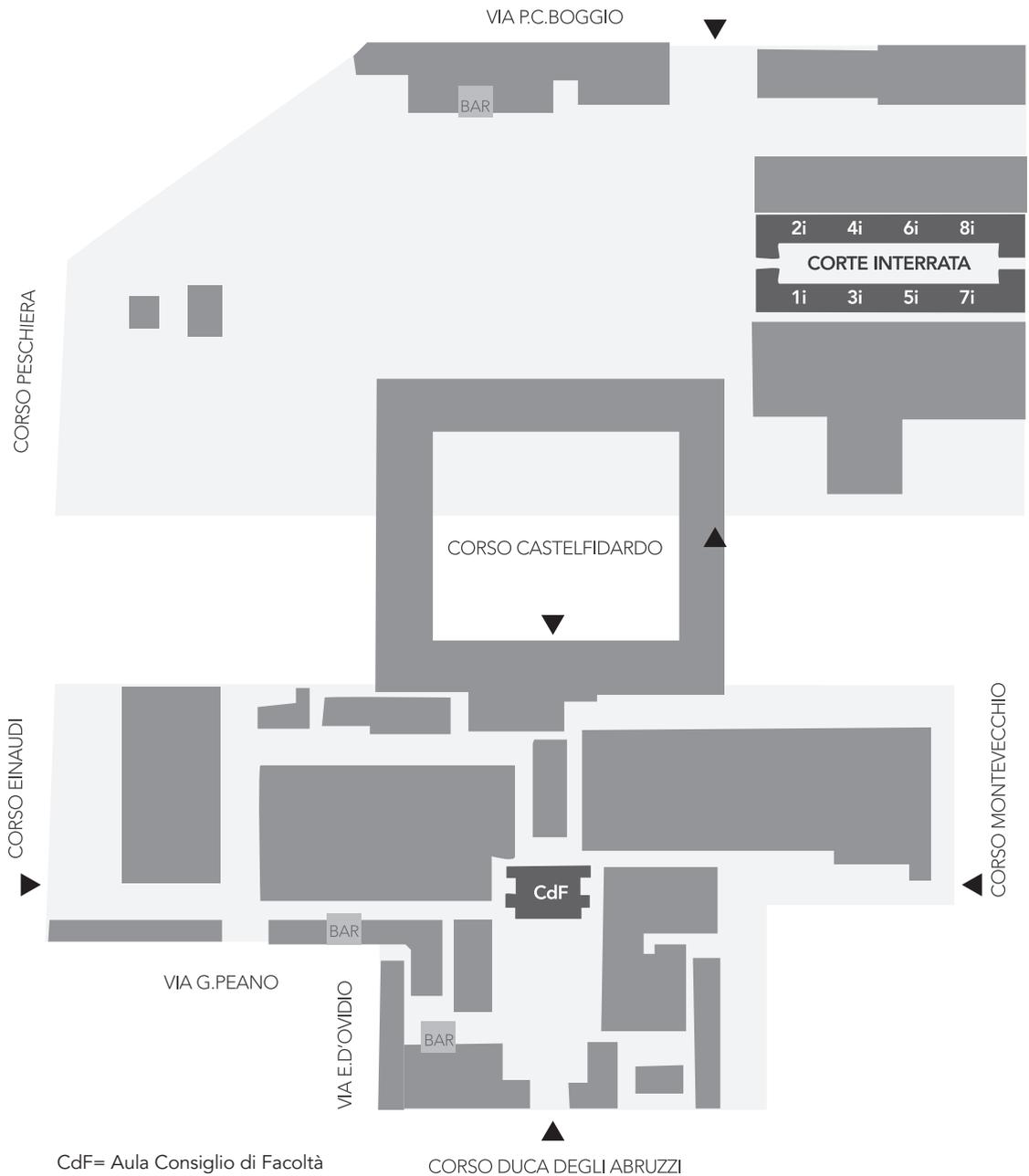
Welcome Drink and Social Dinner Venue:

Ristorante La Magnolia

Via Luigi Mercantini, 6 - Torino

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Room Map



CdF= Aula Consiglio di Facoltà

SIMAI 2012

11th CONGRESS of the
**SOCIETÀ ITALIANA di MATEMATICA APPLICATA ed
INDUSTRIALE**

**ITALIAN SOCIETY for
APPLIED and INDUSTRIAL MATHEMATICS**

Torino, Italy, June 25-28, 2012

ABSTRACTS

Scientific Committee

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Franco Brezzi	IUSS/CNR IMATI, Pavia, Italy
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Roberto Natalini	CNR IAC, Roma, Italy
Luigi Preziosi	Politecnico di Torino, Italy
Luigia Puccio	Università di Messina, Italy

INVITED LECTURES

- Luigi Barletti** Università degli Studi di Firenze, Italy
Quantum fluid models for nanoelectronics
- Paolo Bisegna** Università di Roma Tor Vergata, Italy
Mathematical issues in visual transduction
- Antonio DeSimone** Scuola Internazionale Superiore di Studi Avanzati, Trieste, Italy
Cellular motility: mechanical bases and some mathematical results
- Nicole El Karoui** Ecole Polytechnique, Palaiseau, France
Dynamic utilities and long term interest rates
- Massimo Fornasier** Technische Universität München, Germany
Random dimensionality reduction and sparse recovery algorithms
- Valeria Simoncini** Università di Bologna, Italy
Solution of structured algebraic linear systems in PDE-constrained optimization problems

Quantum fluid models for nanoelectronics

Luigi Barletti

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Quantum fluid equations, which are known since 1926, have recently aroused a renewed interest for their possible applications to the mathematical modeling of nanoscale semiconductor devices. Indeed, they represent an ideal tool for describing the quantum-mechanical behavior of carriers with the advantage of using the "classical" language of fluid-dynamics.

In this talk we present a survey of recent developments in the derivation of quantum fluid equations from an underlying kinetic description. We shall illustrate how the *quantum maximum entropy principle* can be exploited to obtain quantum-fluid models of various kinds and how such models can be semiclassically approximated, which typically leads to equations of Euler or drift-diffusion type with quantum corrections. In particular, we shall focus on systems with spin-like degrees of freedom (KP-model, Rashba spin-orbit, graphene) and systems with indistinguishable-particles statistics (Fermi and Bose fluids). Systems of this kind are expected to play an important role in the future technology.

Perspectives and open problems will be eventually discussed.

Mathematical issues in visual transduction

Paolo Bisegna

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Visual transduction is the process by which photons of light are converted into electrical signals. A highly amplified biochemical cascade is generated in the retinal rod outer segment (ROS) upon absorption of a photon by a G-protein-coupled receptor, thus initiating diffusion of second messengers in the highly-organized cytoplasm of the ROS, to produce a suppression of electrical current flowing into the ROS.

Single photon responses (SPRs) are expected to be inherently variable because the lifetime of a single activated receptor is highly variable, such as the time to decay of a radioactive particle. However, electrophysiological measurements reveal a surprisingly low variability, which is essential for reliably detecting the absorption of single photons. The problem, what mechanism confers the high reproducibility of SPRs, is still open.

A model of the transduction process is presented, accounting for the nanostructure of the ROS. It is based on the theories of homogenization and concentrated capacity and permits a mathematical and numerical analysis of the various interacting components of the process. The model provides an explanation of the reproducibility of SPRs and is applicable to other signaling systems regulated by G-protein-coupled receptors.

Cellular motility: mechanical bases and some mathematical results

Antonio DeSimone

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We will discuss the mechanical bases of cellular motility by swimming and crawling. Starting from observations of biological self-propulsion, we will analyze the geometric structure underlying motility at small scales. We will then illustrate a control-theoretic approach to study the swimming strategies available to microscopic swimmers, and to assess energetic efficiency and optimality of their strokes.

Dynamic utilities and long term interest rates

Nicole El Karoui

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A large debate is open for several years within mathematical finance about the criterion to optimize. A example is given by the forward dynamic utilities introduced by M. Musiela and T. Zariphopoulou in (2003-2010) to model possible changes over the time of individual preferences of an agent. In particular, there is no-prespecified trading horizon. These point of view applied to consumption problem is of large importance in long term decision making. We characterize these dynamic utilities in terms of Hamilton Jacoby Bellman SPEs. An explicit solution is given using monotonic solutions of two stochastic differential equations and their inverse, with a nice interpretation in terms of optimal wealth when these utilities satisfy a property of consistency with a given incomplete financial market. In the controversy on the discount rate used in financing long term projects, such a criterion leads to a yield curve depending of the wealth of the economy.

Random dimensionality reduction and sparse recovery algorithms

Massimo Fornasier
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We start by presenting the optimal dimensionality and complexity properties of an abstract coding-decoding system. The coding of high-dimensional vectors in \mathbb{R}^N is performed by means of a linear map into a lower dimensional space \mathbb{R}^m , where $m \ll N$, and the decoding is performed by means of any nonlinear map with an error proportional to the best k -term approximation. Then we will show that such an ideal and optimal coding-decoding system can be actually realized in practice by compressing high-dimensional vectors into lower dimension via suitable *random matrix embedding* and recovering them by convex optimization, *minimizing the ℓ_1^N -norm* of competitors. We exemplarily present an algorithm to perform efficiently the latter convex optimization, based on iteratively reweighted least squares. We eventually illustrate three variations on the theme, related to applications beyond coding-decoding. First we address uniform approximation algorithms with polynomial complexity to recover high-dimensional functions from random sampling, breaking the curse of dimensionality. Then we propose randomized algorithms to simulate high-dimensional dynamical systems modeling complex interacting agents via multiple projections in lower dimension. We conclude by presenting very recent results in the sparse stabilization and optimal control of such dynamical systems to enforce pattern formation.

Solution of structured algebraic linear systems in PDE-constrained optimization problems

Valeria Simoncini
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Symmetric and indefinite block structured matrices often arise after the discretization of a large variety of application problems, where the block form stems from the presence of more than one partial differential equation (PDE) in the problem, or from an optimization process with constraints, often also involving PDEs. Structure-aware preconditioning strategies have emerged as winning devices for efficiently and optimally solving the associated large linear systems. In this talk we review various forms of symmetric definite and indefinite preconditioners, with special emphasis on PDE-constrained optimization algebraic problems.

YOUNG RESEARCHERS MINISYMPOSIA

YRM 01 - Beyond the mesh: handling geometry with unconventional methods

In the process of the numerical solution of differential problems domain discretization is the first step. However, the complexity that arises in realistic situations is often very challenging for standard discretization methods. Over the last years a wide range of new methods has been developed to tackle complex geometries: mesh-free methods, isogeometric analysis and adaptivity are only a few examples of methods "beyond the traditional mesh". These different approaches have the common purpose of facilitating the simulation of demanding problems that, for instance, exhibit large deformations, contacts and singularities as in the case of mesh-free methods, or that require an exact representation of the geometry which can be guaranteed by the use of NURBS. Moreover the quality of the solution can be improved resorting to different forms of mesh adaptivity such as anisotropic adaptation and hierarchic refinement driven not only by the features of the solution but also by the geometry of the domain. Without claiming to be exhaustive on such a broad subject, this mini symposium aims at presenting the recent developments of a collection of these unconventional techniques with a particular focus on industrial applications in the field of solid and fluid mechanics.

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Franco Dassi

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Anisotropic mesh adaptation for PDE defined on implicit surfaces

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In numerical simulations a lot of applications are related to partial differential equations defined on surfaces: computer animation, design optimization and free surface problems are only a few examples.

In the last years one of the most interesting issue associated with this topic is mesh adaptivity, in particular anisotropic mesh adaptation. In order to proceed with this kind of process, we need to derive a suitable anisotropic estimator that will drive the adaptation process, but it is not a trivial task. In the classical setting, where the differential problem is solved in a plain domain, the error estimator involves only the information related to the finite element approximation of the problem. On the contrary, in our context the error estimator should take into account also the approximation of the surfaces. Actually it will consist of two different contributions [2] [3]:

- an *almost-best-approximation term*, typical of a finite element discretization;
- a *geometric error term*, due to the discretization of the surface.

Moving from this estimator, we aim at devising a mesh modification process (such as node smoothing, edge collapsing [1] [4]) applied to a discretization of the surface with the final goal of improving the accuracy of the discrete solution.

1. Gruau C. and Coupez. T. Comput. Methods Appl. Mech. Engrg. 2005 *3d tetrahedral, unstructured and anisotropic mesh generation with adaptation to natural and multidomain metric.*
2. Dziuk. G. Partial Differential Equation Calc. Var. 1988 *Finite elements for the beltrami operator on arbitrary surfaces.*
3. Mordin P. Mekchay K. and Nochetto R. Mathematics of Computation. 2011 *Afem for the laplace-beltrami operator on graphs: design and conditional contraction property.*
4. Micheletti S. Farrell P.E. and Perotto S. To appear in Int. J. Numer. Methods Engrg. 2011 *An anisotropic zienkiewicz-zhu type error estimator for 3d applications.*

Optimal transformation mesh-free method: a mesh-free method for solid and fluid flows

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Mattia Penati

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The Eulerian framework for the description of fluids and solids becomes inconvenient when variable domains and topological transitions, like fractures, are involved. In order to overcome these difficulties a large number of numerical techniques has been developed, including meshfree methods. Most of these schemes are based on the construction of a partition of unit without the requirement of a polygonal mesh, but only a material point sampling is needed. Among these the maximum entropy approximation is the only ensuring a weak Kronecker-delta property at the boundary: this property allows an easier enforcement of essential boundary conditions and the coupling with finite elements methods. Optimal transportation meshfree (OTM) method combines concepts from optimal transportation theory and maximum entropy approximation. The idea behind this method is to use the max-ent approximation as a basis for the numerical solution of problems governed by a minimum principle. In this way mass transport and essential boundary conditions are enforced exactly and linear and angular momentum are conserved. Some applications for fluids and elastic solids will be shown to assess the properties of OTM method; moreover the OTM method will be compared with the finite elements methods.

1. Arroyo, M. and Ortiz, M. 2006 Local maximum-entropy approximation schemes: a seamless bridge between finite elements and meshfree methods. *International Journal for Numerical Methods in Engineering* 65, 2167–2202
2. Li, B., Habbal, F., and Ortiz, M. 2010 Optimal transportation meshfree approximation schemes for fluid and plastic flows. *International Journal for Numerical Methods in Engineering* 83, 1541–1579

An approach to local refinement in isogeometric analysis: LR-splines

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Isogeometric analysis is a framework in which the simulation is done on the exact geometry. This is achieved through parametrization of the domain. In isogeometric analysis the approximate solution is searched in a finite dimensional space based on B-splines that is related to the parametrization map. This choice permits the use of smooth functions that have better approximation properties.

On the other hand B-splines are linked to a tensor product structure of the mesh and thus local refinement is difficult. Many possible solutions have been proposed: hierarchical-splines (1988), T-splines (2003), PHT-splines (2008) and LR-splines (2012) [1]. The focus here is on LR-spline properties. In particular how to represent polynomials, the number of non zero generators at each point (that influence the sparsity of the mass matrix) and linear independence.

1. Dokken T., Lyche T. and Pettersen H. F. 2012 Locally refinable splines over box-partitions. In SINTEF ICT

Automatic, hierarchic and adaptive mesh generation on CAD surfaces for BEM simulations of ship hydrodynamics

Antonio DeSimone

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We present an automatic mesh generation methodology for the simulation of three dimensional unsteady and nonlinear waves generated by a ship advancing in water [1]. The governing potential flow equations are discretized by means of the Boundary Element Method (BEM), which only requires the generation of surface meshes. At the simulation start, the specific CAD model of the hull (consisting in an IGES or STEP file) is imported. An initial mesh, composed of a small set of elements, is first generated. Hierarchic and non conformal mesh refinements are then performed placing new points in high curvature regions of the hull, until user specified quality requirements are met. During the simulation the mesh is then deformed to track the motion of the free surface around the boat, and is adaptively refined via a posteriori error estimator. Mesh generation and deformation, along with BEM discretization of the flow equations has been implemented employing the open source C++ library deal.II [2], while interface with the CAD model of the hull relied on the open source OpenCascade C++ library. Preliminary results are presented where we compare numerical results with experiments on the case of a hull advancing in calm water with fixed sink and trim.

1. Mola A., Heltai L., DeSimone, A. *A stable and adaptive semi-lagrangian potential model for unsteady and nonlinear ship-wave interactions*. Technical Report 06/2012/M, SISSA, 2012.
2. Bangerth W., Hartmann R., Kanschat G. *deal.II a general purpose object oriented finite element library*. ACM Transactions on Mathematical Software, 33(4):24/124/27, 2007.

YRM 02 - Mathematical models for renewable energy sources

In recent years, scientific research on sustainable energy has become a pressing and relevant topic. However, the idea to look at the problems from an applied mathematics point of view is still quite new, despite it being fundamental for further developments.

Classical tools from applied mathematics can be applied across a large variety of applications concerning renewable energy. This collection of talks propose three examples of mathematical modelling for renewable energy power sources and a study of future uptake of renewable energy technologies based on a mathematical model of incentive schemes.

The first talk concerns parabolic trough power plant technology, which utilizes solar energy in large power plants. It presents a mathematical model for heat and mass transfer in parabolic trough power plants and describes a suitable numerical code used to compare the performance of the different kinds of heat transfer fluid.

The second proposed talk, examines four renewable energy incentive schemes designed to boost growth of sustainable electricity production. It presents a generalized mathematical model of industry growth, fitted with data from the UK onshore wind industry. The model is developed to calculate the optimal strategy for provision and timing of subsidy for each scheme. Finally, a comparison of the performance of each scheme is presented.

Our third speaker analyses the air dynamics inside solar chimney power plants in the special case of high latitudes. The results obtained from numerical simulations are compared to experimental data relative to three high latitude locations in Ottawa, Winnipeg and Edmonton in Canada.

Finally, the fourth talk proposes a model for Osmotic power plants. The development of this particular kind of renewable energy source has found recent application at the Norwegian company Statkraft, but there is still scope for mathematical modelling. The talk presents a first attempt to analyse a stationary model on which perform numerical simulations.

Organizers:

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Mathematical modeling and simulations of parabolic trough power plants

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Parabolic trough power plants is a technology for utilizing solar energy in large power plants. These use curved, long, parabolic mirrors that focus the sun's direct beam radiation on a linear receiver tube located on the focus of the parabola. This tube contains a heat transfer fluid (HTF), that is heated and it is used to generated superheated steam. At the final step the superheated steam is transformed into electricity by using a reheat steam turbine-generator. Different kinds of HTFs are now available:

1. Oil
2. Ionic fluid
3. Water and steam

In this talk we show a simple mathematical model for heat and mass transfer in parabolic trough power plants. We also present a suitable numerical code, by use of which we compare the performance of the different kinds of transfer fluid, in order to understand which provides the best performance.

Renewable energy incentive schemes: performance comparison using optimal control

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In order to meet renewable energy targets, many governments have instituted incentive schemes for renewable electricity producers. These schemes aim to boost investment and hence growth in renewable energy industries. Our work examines four such schemes: premium feed-in tariffs, fixed feed-in tariffs, feed-in tariffs with contract for difference and the renewable obligations scheme. We present a generalised mathematical model of industry growth, and fit the model with data from the UK onshore wind industry. We develop the model to respond to subsidy from each of the four incentive schemes, and thereby calculate the optimal strategy for provision and timing of subsidy for each scheme. Finally, we present a comparison of the performance of each scheme, given that they use their optimal control strategy.

A 1-D model for pressure retarded osmosis

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The possibility of energy production through osmosis between river and ocean water is well known since several years, and recently the Norwegian company Statkraft (www.statkraft.com) started developing a power plant based on the concept of pressure retarded osmosis. Such process relies on the fact that sea water, pressurized to a pressure p between the environmental and the osmotic pressure of the sea water itself, $(p - p_E) < p_{osm}$, draws fresh water at the environmental pressure p_E through a semipermeable membrane. This increases the flow of pressurized brackish (lower salt content than seawater) water, which is split into two streams. The first stream runs through a turbine to produce power, while the other stream is used to pressurize the incoming seawater in a pressure exchanger. The aim of this talk is to present a first attempt to analyse a stationary model for pressure retarded osmosis on which perform numerical simulations.

Mathematical modeling and simulation of solar chimney power plants for high latitudes

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The gas (air) dynamics inside solar chimney power plants with sloped collector field were studied. A 1D approach was taken to construct underlying mathematical model to describe the gas (air) dynamics. Derivation of model entailed inclusion of relevant source and sink terms in fully compressible system of Euler equations of gas dynamics. The model adequately describe the main features of physical effects involved. The model was subject to so called low Mach number asymptotics, then the numerics were performed. Therefore, the overall approach is a compromise between pure qualitative and pure quantitative analysis. A code was developed in MATLAB to obtain simulation results e.g. velocity, density and temperature profiles for three realistic high latitude locations at Ottawa, Winnipeg and Edmonton in Canada.

YRM 03 - Numerical resolution of PDE: the potentiality of the LifeV library

The LifeV finite element library, developed over the last years by Politecnico di Milano, Emory University, EPFL and INRIA, is a powerful tool for the numerical solution of PDE. It implements state of the art numerical methods such as non linear solvers, multiscale approach, Mixed Finite Elements, Newmark time integration schemes and a lot of preconditioning techniques, serving both as a research and a production library. One important feature that makes this library one of the most powerful open source Finite Elements codes among the others is its parallel nature. In fact the code has been developed based on the most advanced parallel libraries like Trilinos, for linear algebra algorithms, and ParMetis, for partitioning of the mesh. In this manner LifeV can handle problems characterized by a huge computational cost. The range of application of LifeV is very wide, indeed it deals with physical problems that vary from the geological to the biomedical framework. These series of talks will focus only on a small set of problems that LifeV can solve, they will underline its good performance without going into detail about technical and implementative aspects of the code.

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An isogeometric analysis module for LifeV

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Iso Geometric Analysis (IGA) [Hughes, Cottrell, Bazilevs, 2005] is an approximation method for Partial Differential Equations whose main feature is the ability of maintaining the same exact CAD-based description of the computational domain geometry throughout the analysis process, including refinement. A common choice in the framework of IGA is that of relying on the isoparametric approach which consists of using the same basis functions, usually Non-Uniform Rational B-Splines (NURBS), for both the geometry description and the approximation of the unknown solution fields. Even in cases where the isoparametric approach is not used, NURBS based approximations have been shown to provide several advantages over Finite Elements in terms of accuracy and computational efficiency. In this talk, we describe a prototipal implementation of an IGA solver module for the finite elements library LifeV. The module provides the ability to import into LifeV geometry and function space data structures exported by the IGA Library GeoPDEs [de Falco, Reali, Vazquez 2011]. We discuss the design of the LifeV IGA module, and the implementation issues related with its integration into the existing structure of the LifeV Library. Preliminary examples of benchmark problems on nontrivial geometries are presented.

An XFEM method for 3D elliptic interface problems

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In numerical simulations of phenomena with pronounced non-smooth characteristics, a new class of methods has been recently developed. These methods, named XFEM (Extended Finite Element Methods), allow for discontinuities internal to the elements of the mesh. A local enrichment of the standard approximation space is the basis of XFEM. The choice of shape and localization of enrichment functions generates a large variety of methods, that can be exploited in several industrial applications. The XFEM method proposed in [1] has been implemented in LifeV to solve elliptic interface problems in a 3D domain. This method has been extended in order to handle more than one discontinuity interface. Domain is divided in regions with respect to the sign of level-set functions whose zero-levels are interpreted as the discontinuity interfaces. We are interested in solving problems in which the diffusion and reaction coefficients depend on the region of the domain. Theoretical estimates about convergence of the method are compared with numerical results and the performances of the parallel code are analysed.

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Numerical modeling of sedimentary basin evolution on HPC systems

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In this talk we address the numerical modeling of a sedimentary basin geological evolution using the LifeV finite element library, focusing on high performance computing (HPC) performance.

The mathematical model that we present assumes that different rock types can be considered as homogeneous layers that are immiscible and undergo a creeping flow in a Stokes regime during geological ages. Physical constants, such as viscosity and density, are constant in each subdomain. Interfaces between different layers are tracked in order to reconstruct the concentration of the different rock species in each point of the domain.

From the numerical point of view, typical basin dimensions are in the range of few kilometers in each direction and a realistic geometry requires a high resolution unstructured grid to properly capture the evolution of the rock layers. The discretized system therefore introduces matrices with a number of lines in the order of the million. The solution of such problems greatly benefits from an effective parallelization of the solver.

Simulating electromechanical coupling in the heart

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The muscles, and the heart in particular, can be seen as active materials, because they can undergo deformations in absence of external loads: a thermodynamical system able to spend energy at the microscale in order to produce work at the macroscale. This characteristic is usually introduced into the continuum mechanic formulation with a additional stress term, that depends on the internal dynamic, that typically involves calcium ions, and the deformation itself [2]. A less popular approach, addressed also in this talk, takes into account a Lee-type multiplicative decomposition of the strain [1,3]. The muscle contraction is controlled by a travelling electric wave, produced by selfexcitable cells specifically located, that initialize and synchronize the mechanical activity. In particular, the electric potential triggers a release of calcium ions throughout the intracellular space. It is also well known that contraction mainly occurs in fibers direction, although it has become evident from experiments that a non-negligible amount of the activation occurs also in cross-fiber direction. Numerical approximation of the heart activity poses intriguing questions, mainly because of a strong link between electrophysiology, that activates the muscle, mechanics and circulatory system, from which boundary conditions are provided.

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YRM 04-05 - Reduced and polynomial approximation strategies for parametrized and stochastic PDEs I - II

Problems modelled by PDEs depending on a set of parameters arise in different areas of applied mathematics and engineering. Relevant examples are control/optimization of complex systems, computation of statistics for systems with stochastic parameters and inverse problems.

From a computational point of view, these problems require an efficient approximation of the dependence of the PDE solution from the set of parameters. Several reduced approaches (based on interpolation, projection, regression) are available, and require the repeated solution of the PDE for a set of sampled parameters values. Efficient sampling may be an additional challenge, given the usual high dimensionality of the parameter space.

The aim of this minisymposium is to bring together young researchers coming from different research areas and developing different strategies to tackle these topics. A non-limiting list of strategies fitting to this minisymposium includes e.g. sparse grids, reduced basis, collocation methods, polynomial chaos, proper orthogonal/generalized decomposition.

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Computational and geometrical reduction strategies for parametrized fluid dynamics equations

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Despite the computer resources nowadays available, it is still difficult to deal with applications and scenarios involving the repeated solution of PDEs on different data settings (many-query context). For instance, the most common numerical strategies used to tackle optimal control, shape optimization and inverse problems under PDE constraints are based on iterative optimization procedures, involving several input/output evaluations and PDE solutions. With this respect, reduced order modelling can represent a suitable strategy to allow for the solution of these problems, entailing an acceptable amount of CPU time and limited storage capacity.

Our framework developed to address inverse problems in fluid dynamics - such as flow control, shape optimization, inverse identification problems - is based on the coupling between suitable (control, shape, etc.) parametrization strategies and the reduced basis method for parametrized PDEs. We review the current state of the art of the reduced basis method for fluid dynamics equations, with a special emphasis on a posteriori error estimation in the Stokes and Navier-Stokes equations in parametrized geometries obtained by means of volume-based shape parametrizations.

Numerical examples dealing with inverse problems arising in haemodynamics are presented in order to show the capabilities of our reduced framework.

The reduced basis method for nonlinear elasticity

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Many elastic phenomena in structural mechanics undergo small deformations and can be described by linear equations. On the other hand, problems involving large displacements or rotations (cables, beams or shells) present a nonlinear behavior and require an exact geometric treatment. The latter means that the *reference* undeformed configuration and the *current* deformed configuration cannot be equalized, unlike in the case for linear elasticity. So far the literature on model order reduction for nonlinear elasticity is scarce: Although methods like the Proper Orthogonal Decomposition may be promising, nonlinear dependencies represent a serious drawback. Thus, issues and challenges in applying the Reduced Basis Method [2] for problems in nonlinear elasticity are discussed. Through a Galerkin projection, the RB Method replaces a Finite Element model with a low-dimensional RB model. Preliminary results are presented for two cases: A first example is a buckling problem [1] for a compressed 2D column, where the trivial linear solution becomes unstable in correspondence to a critical load. The instability load and displacement are identified through an eigenvalue problem. A second example deals with the choice of the constitutive relation characterizing the elastic material response [3]: A St. Venant linear relation is accepted for many engineering applications, whereas a hyper-elastic relation, such as Neo-Hooke, is physically more precise, though introducing higher order nonlinearities.

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Approximation of quantities of interest in stochastic PDEs by the discrete L^2 projection on polynomial spaces with random evaluations

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In many PDE models the parameters are not known with enough accuracy and can be treated therefore as random variables. The challenge is then to efficiently compute the law of the solution of the PDE or some Quantities of Interest, given the probability distribution of the random input parameters.

We look for a multivariate polynomial approximation ([1],[2]) of the parameter to solution map.

In [3] we consider univariate or multivariate functions and study the approximation properties of the random L^2 projection with respect to the number of sampling points, the maximum polynomial degree, and the smoothness of the function to approximate.

We prove optimality estimates (up to a logarithmic factor) when the random points are sampled from bounded random variables with strictly positive probability density functions. Our analysis of the random projection proves that the optimal convergence rate is achieved when the number of sampling points scales as the square of the dimension of the polynomial space. Moreover, it gives an insight on the role of smoothness and the conditioning of the random projection operator in the stability of the L^2 projection.

In this talk we will present the application of this methodology to compute Quantities of Interest associated to the solution of PDEs with stochastic coefficients and with random domains.

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Polynomial chaos decomposition for differential models including technology variability

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Nowadays, the numerical simulation of circuits and their interconnections is a fundamental step in the design phase due to the urging necessity to perform right-the-first-time designs. In this regard, several analysis tools are available, although they are usually deterministic and this represents a strong limitation whenever manufacturing tolerances or uncertainties on design parameters cannot be neglected. In this framework, the stochastic analysis is a tool that is extremely useful in the early design phase for the prediction of the actual system performance and for setting realistic design margins. These structures are described by differential equations and the typical resource allowing to collect quantitative information on the statistical behavior of the circuit response is usually based on their sampling according to the brute-force Monte Carlo (MC) method. Such method, however, requires a large number of samples, thus often becoming computationally prohibitive. Recently, an effective solution that overcomes the previous limitation has been proposed. This methodology is based on the polynomial chaos (PC) theory and on the representation of stochastic partial differential equations in terms of orthogonal polynomials. The authors of this contribution proposed an application of PC theory to the analysis of electronic circuits and, in particular, of distributed structures described by transmission-line equations.

Polynomial approximation of stochastic PDEs

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Partial differential equations with stochastic coefficients are a suitable tool to describe systems whose parameters are not completely determined, either because of measurement errors or intrinsic lack of knowledge on the system.

We consider here the case of elliptic PDEs, in which the state variables usually exhibit high regularity in their dependence with respect to the random parameters. It is therefore sound to introduce a global polynomial approximation over the stochastic space for the state variables and their statistical moments (“Sparse Grid Stochastic Collocation Method”).

When the number of parameters is moderate, this method can be remarkably more effective than classical sampling methods. However, contrary to the latter, the performance of the sparse grid approximation deteriorates as the number of random variables increases (“Curse of Dimensionality”); to prevent this, care has to be put in the construction of the approximating sparse grid.

In this talk we will show that the construction of a sparse grid can be reformulated as a classical knapsack problem over the tensor interpolant operators forming the sparse grid. We will solve the knapsack problem thanks to a-priori estimates of the profit of each operator, and show numerically the effectiveness of the sparse grids thus obtained.

Uncertainty propagation through polynomial chaos expansion of a sedimentary basin compaction model

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Basin scale compaction is driven by mechanical compaction and geochemical processes. These mechanisms are associated with large characteristic spatial and temporal scales. In this context, estimates of the parameters included in predictive models are affected by considerable uncertainty. Here, we consider the impact of model parametric uncertainty on the prediction of the model outputs. The system is characterized through a one-dimensional numerical model which we approximate through a Generalized Polynomial Chaos Expansion (GPCE), implemented via a sparse grid sampling in the selected parameters space. The GPCE is employed to perform uncertainty propagation studies grounded on a Monte Carlo analysis of the system. The properties of the GPCE allow straightforward evaluation of the variance-based Sobol indices. These provide a quantification of the way parametric uncertainty propagates to system states. Results are illustrated through a one-dimensional example, involving mechanical compaction and quartz cementation in sandstones. The methodology employed allows to characterize the probability density function of the output state variables in multiple locations, to identify the main interactions amongst the parameters affecting pressure, temperature and porosity distributions. It can also be efficiently embedded within an inverse modeling of the compaction process.

Reduced basis method for parametrized optimal control problems

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We present the development, analysis and computer implementation of a suitable model reduction paradigm – the reduced basis (RB) method – for the rapid and reliable solution of parametrized optimal control problems governed by PDEs. In particular, we develop the methodology for parametrized quadratic optimization problems with either coercive elliptic equations or Stokes equations as constraints. Firstly, we recast the optimal control problem in the framework of saddle point problems in order to take advantage of the already developed RB theory for Stokes-type problems. Then the usual ingredients of the RB methodology are provided: a Galerkin projection onto a low-dimensional space of basis functions properly selected by an adaptive procedure; an affine parametric dependence enabling to perform competitive Offline-Online splitting in the computational procedure; an efficient and rigorous a posteriori error estimation on the state, control and adjoint variables as well as on the cost functional. Finally, the reduction scheme is applied to several numerical tests confirming the theoretical results and demonstrating the efficiency of the proposed technique.

Reduced models For data assimilation in haemodynamics

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Mathematical models and numerical methods for fluid dynamics have both experienced a terrific improvement in the last 25 years. However, they often still use coefficients taken from literature or basal medical values. On the other hand, also medical imaging devices have experienced a tremendous improvement in the last 25 years. Still, the acquired images are affected by noise. Data Assimilation (DA), a technique already used in other fields, like meteorology, aims to include the information coming from data inside the mathematical model, in order for achieve more accurate and reliable results. Thanks to the improvements mentioned above, is now possible to apply this paradigm to haemodynamics problem, in order to provide more accurate and reliable estimates of some quantity of interest (wall shear stress, vessel compliance, etc.). Here we present one application of DA and the variational approach we used to solve it, together with some results. Since the complexity of the optimization problem arising from the incorporation of the measures in the model demands for a reduction of the computational costs, we finally introduce a Reduced Basis approach together with some results.

MINISYMPOSIA

MSP 01-03 - Advances in numerical methods and applications I - II - III

Scientific Computing is becoming an essential element of every branch of science and technology, driven by the vast amount of experimental data requiring analysis, and the need for increasingly realistic simulations of ever more complex systems. Then, there is a high demand for efficient and reliable numerical algorithms for solving important problems.

This minisymposia deals with some recent computational approaches including both analysis and advanced applications in industrial and scientific problems. Topics involve numerical solutions of ordinary differential equations, Galerkin methods for partial differential equations, Approximation Theory, inverse problems, Optimization Theory. Applied Scientific Computing problems include Digital Image Processing, Neural networks, Shape Optimization, packaging applications, multiscale problems, and partial differential equations with a complex geometrical domain. Finally, both deterministic and statistical (and stochastic) approaches appear in some applications.

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Approximated nonstationary iterated Tikhonov with application to image deblurring

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In this talk we present new iterative regularization methods, based on the approximation of nonstationary iterated Tikhonov. In particular we investigate the image deblurring problem, where the blurring matrix is not easily invertible with a low computational cost, while an approximation with such property is available. This is for instance the case of block Toeplitz matrices with Toeplitz blocks that can be well approximated by block circulant matrices with circulant blocks matrices which can be diagonalized by two dimensional fast Fourier transforms. Matrices arising from the imposition of other boundary conditions can be considered as well. A detailed analysis is proposed in the stationary case and we discuss relations with preconditioned Landweber method and other known methods. A large numerical experimentation with different boundary conditions, blurring phenomena and noise level is presented.

Approximation by sigmoidal functions and applications

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Neural networks have been widely used in Approximation Theory. In 1989, G. Cybenko gave in [1] a non-constructive proof that every continuous function on $I := [0, 1]$ can be uniformly approximated by neural networks like

$$\sum_{k=0}^N \alpha_k \sigma(w_k x - x_k), \quad x \in I, \quad \alpha_k, w_k, x_k \in \mathbb{R},$$

where σ , the “activation function” of the network, is a *sigmoidal function*, i.e., a real-valued function such that $\lim_{x \rightarrow -\infty} \sigma(x) = 0$, $\lim_{x \rightarrow +\infty} \sigma(x) = 1$. We have developed a *constructive* theory for approximating functions of one or several variables, even uniformly and in L^p , by superposition of sigmoidal functions, on bounded domains. A simultaneous approximation, with the same order of accuracy, of a given function and its derivatives (whenever they exist), is also obtained. Applications boundary-value problems for ODEs were shown.

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Constrained nonlinear optimization for parameters identification in imaging

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In this talk we consider a separable nonlinear least squares framework to model and solve parameters identification in imaging. Since imaging applications are severely ill-posed, regularization techniques are necessary in order to obtain a meaningful solution. We show that, by imposing opportune constraints on the variables and with well chosen regularization parameters, it is possible to obtain a fairly well behaved objective function. Thus the resulting nonlinear minimization problem can be effectively solved by classical methods, such as Gauss-Newton algorithm.

In particular we show the numerical results of an application to blind deconvolution, modeled as a separable problem, where the unknowns can be distinguished between linear and nonlinear variables. The nonlinear parameters to be identified are the variables describing the Point Spread Function, while the linear unknowns are the image to be restored. Nonnegative constraints are imposed on the linear variables. We show that the constrained formulation of the blind deconvolution problem provides better results than the unconstrained case.

Shape parametrization and computational reduction for real-time simulations in varying geometries

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Many problems in scientific computing, such as shape optimization [4], shape registration [5], and more general inverse problems [1], are formulated on parametrized domains.

We review some flexible and general methods used to represent shapes, either implicitly or explicitly, with a special emphasis on choosing methods that can be combined with existing model reduction approaches for PDEs. We present techniques developed recently for treating the complexities related to model reduction of PDEs on varying domains. Two different approaches may be considered: free-form deformations [3] and radial basis functions [5]. In both cases the problem is reduced to a fixed mesh with parameter-dependent coefficients, allowing us to apply the reduced basis method. Some remarks regarding the optimal choice of the shape parametrization will also be presented in view of reducing the parametric dimension of the problem to a more tractable one.

Numerical examples of the proposed techniques are presented for the rapid solution of shape-related inverse-like problems [2].

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A statistical-numerical approach for surface fitting over non-planar domains

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We propose a new approach for accurate surface fitting over non-planar bi-dimensional domains. In particular, we are interested in surface domains embedded in a three dimensional space. Our approach essentially consists of two phases: first we conformally map the original surface domain to a region in \mathbb{R}^2 then existing spatial smoothing techniques for planar domains that are suitably modified to account for the domain deformation are applied. For smoothing, the surface estimate minimizes a penalized sum of squared error functional where penalty consists of the L^2 -norm of the Laplace-Beltrami operator of the original non-planar domain. An interesting contribution of our approach is the merging of statistical and numerical techniques. Indeed the finite element approach is employed to approximate both the conformal flattening map and the error functional. The method is particularly well suited for fitting large amounts of experimental data. The driving application of the proposed approach is the modeling of hemodynamic data, such as wall shear stress or blood pressure, for instance on the wall of a carotid artery.

Equations for the probabilistic moments of the solution of SPDEs

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Annalisa Buffa

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The boundary value problems for PDEs which model many natural phenomena and engineering applications are affected by uncertainty in the input data. One way to effectively address this issue is to describe the problem data as random variables or random fields, so that the deterministic problem turns into a stochastic differential equation (SPDE). The solution of a SPDE is itself a random field with values in a suitable function space.

The simplest approach is Monte Carlo Method. Generally, its convergence rate is slow, so that this method turns to be costly. An alternative technique is to derive the moment equations, that is the deterministic equations solved by the probabilistic moments of the stochastic solution. See for example [3,4] and the references therein for problems with stochastic loading terms and [2] for problems with stochastic domains.

We take into account steady state linear stochastic partial differential equations. We consider both cases of elliptic equations with stochastic loads and random coefficients. Given complete statistical information on the random input data, the aim of our work is to compute the statistics of the random solution.

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The L^2 -projection in the spatial discretization of heat equations

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We analyze Galerkin approximation in space of the heat equation with particular attention to quasi-optimality, in the sense of Cea's Lemma. The error norms we consider are associated to the standard weak formulation of parabolic problems. In this setting, quasi-optimality has been derived in [2] for a mesh-depending norm close to the one of $H^1(H^{-1}) \cap L^2(H^1)$. Other works in this direction are [1] and [3], which require the additional assumption of the H^1 -stability of the L^2 -projection onto the discrete space. Under this hypothesis, quasi-optimality in $H^1(H^{-1}) \cap L^2(H^1)$ and stability in $L^2(H^1)$ have been established in [1] and [3], respectively. By means of the inf-sup theory, we unify the existing results and reveal that this hypothesis is also necessary. More precisely, we show that the results in [1] and [3] are essentially equivalent, and that [2], together with the H^1 -stability of the L^2 -projection implies quasi-optimality in $H^1(H^{-1}) \cap L^2(H^1)$. As application, we consider the finite element approximation in space and derive a priori error bounds in terms of the local meshsize that are of optimal order under minimal additional regularity.

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A RKDG scheme for 2D SWE on curved boundary domains

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This work regards a high-order numerical scheme for the integration of the two-dimensional Shallow Water Equations (SWE). First, we highlight the importance of the high-order representation of the boundaries when the numerical scheme has a high-order accuracy. We show the impossibility to obtain a physically realistic solution for some families of steady-state problems using only straight-sided elements [1]. Moreover, we prove that the existing techniques are not suitable to obtain a well-balanced model for curved boundaries.

Our solution to the examined problems consists of a third-order-accurate, well-balanced, Runge-Kutta discontinuous Galerkin (RKDG) model [2] for the integration of the SWE on an unstructured triangular grid. The problem of the curved boundary is addressed by using a proper mixture of straight-sided elements, in the inner part of the computational domain, and of elements with a single curved edge, in the regions near the boundaries [3].

A careful combination of available techniques yields a well-balanced model on the straight-sided elements, and an original approach is proposed for balancing the model on the curved-sided elements. This approach is based on a modified mathematical model of SWE which is consistent with the original one and allows to achieve the well-balancing property.

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XFEM for Darcy problems with networks of fractures

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Porous media flows are influenced by the presence of fractures, *i.e.* strong and localized heterogeneities of the medium, which can act as preferential paths or barriers. The authors in [2] have developed a model to handle fractures as objects of dimension $N - 1$ in domains of dimension N in the case of non-matching grids using the XFEM, see [1]. We enrich the reduced model and the XFEM to the case of intersecting fractures. The grids of the fractures can be independent, increasing the applicability of the scheme to problems with complex geometries such as oil migration in fractured basins or pollutant dispersion in groundwater flows.

1. Carlo D'Angelo and Anna Scotti 2011 A Mixed Finite Element Method for Darcy Flow in Fractured Porous Media with Non-Matching Grids. In *Mathematical Modelling and Numerical Analysis*
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Subsoil decontamination with bioventing: numerical experiments

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A mathematical model describing the bioventing technique for the decontamination of polluted subsoil will be presented. Bioventing is a biological technique: bacteria remove the contaminant transforming it and oxygen is consumed in the reaction. The numerical model is based on the fluid flow theory in porous media and bacteria population dynamics and it describes: pollutant degradation, oxygen and bacteria concentration. The mathematical model will be numerically solved and the results of some experiments will be presented.

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Multi-scale numerical models for fluid-structure interaction problems in packaging applications

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The forming process of a carton-based package for liquid food is a very difficult physical problem to simulate, in particular due to the strong interaction between the packaging material tube and the filling fluid. During the package forming, the cross-section of the carton tube changes abruptly, generating strong pressure waves which propagate along the tube and interact with the other system components. To solve this complex fluid-structure interaction problem, we have developed a set of numerical tools based on both partitioned and monolithic FSI couplings. We discuss the stability properties of the different FSI algorithms that have been considered and we show the role that a geometrical multi-scale (1D/3D) coupling can play in this kind of problems. We present the numerical results of several simulations that have been performed with both 1D and 3D models, as well as some relevant test cases to validate the 1D/3D coupling through the geometrical multiscale approach.

Discontinuous Galerkin approximation of relaxation models for nonlinear diffusion equations

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We present finite element approximations of relaxed systems for nonlinear diffusion problems, which can tackle also the cases of degenerate and strongly degenerate diffusion equations. Relaxation schemes take advantage of the replacement of the original partial differential equation with a semi-linear hyperbolic system of equations, with a stiff source term, tuned by a relaxation parameter ϵ . When $\epsilon \rightarrow 0^+$, the system relaxes onto the original PDE: in this way, a consistent discretization of the relaxation system for vanishing ϵ yields a consistent discretization of the original PDE. The advantage of this procedure is that numerical schemes obtained in this fashion do not require to solve implicit nonlinear problems and possess the robustness of upwind discretizations. The proposed approximations are based on a discontinuous Galerkin method in space and on suitable implicit-explicit integration in time. Then, in principle, we can achieve any order of accuracy, and obtain stable solutions, even when the diffusion equation becomes degenerate and solution singularities develop. Some preliminary theoretical results are given and several numerical tests in one and two space dimensions, both for linear and nonlinear diffusion problems, including a degenerate diffusion equation.

**MSP 04-05 - Approximation methods for data and image
processing
I - II**

Recently, the executive board of SIMAI approved the activation of the SIMAI-SIMA (Signals, Images, Modeling and Approximation) Activity Group, 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. This minisymposium is intended to formalize the beginning of the activities of such group and to give the opportunity to present recent results on some of the aforementioned topics.

In particular, the eight talks included in the minisymposium present research advances both in the theoretical aspects related to the construction of suitable mathematical models for data analysis (wavelets, radial basis functions, box-splines) and in the application of approximation methods to data processing problems (bioimages and keratography maps analysis, image reconstruction and registration, watermarking).

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Statistical and deterministic methods for image reconstruction in X-ray solar astronomy

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Solar hard X-ray imaging cannot be performed by means of focused optics, but rather using image modulation. Therefore raw data do not reveal the image immediately, but only after processing. A traditional approach to image reconstruction implies the deconvolution of a *dirty map* of the event by means of some regularization method that reduces the blurring effect of collimators. An alternative, more sophisticated approach, is tailored to the specific way in which Rotating Modulation Collimators encode imaging information. Indeed each X-ray collimator-detector pair provides a temporal modulation of the arriving flux which can be reduced to a specific set of spatial Fourier components of the source. These data, the purest form of the X-ray telescope data stream, are called *visibilities* and are calibrated measurements of specific spatial Fourier components of the emitted radiation field.

In this talk we describe several deterministic and statistical approaches to image reconstruction from X-ray dirty maps and visibilities and discuss their effectiveness in the case of measurements provided by the NASA *Reuven Ramaty High Energy Solar Spectroscopic Imager* satellite. The impact and reliability of such methods will be assessed also in the framework of a future ESA mission that will provide visibilities characterized by an unprecedented signal to noise ratio.

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A high capacity fragile and reversible medical image watermarking method

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Data hiding has been focusing in medical applications in the last years. In particular, fragile reversible watermarking is a feasible technique when safety aspects including authentication, compliance testing, and guarantee of privacy for sensitive data are key issues [1]. This work proposes a data hiding scheme to guarantee all above features for radiographic images transferred through a generic transmission channel. In particular the mentioned scheme covers the combined use of digital signature techniques and fragile reversible watermarking in the spatial domain in order to embed the patient data and the digital signature in the original image: high capacity and visual quality are ensured. The authors have analysed a large set of radiographic images in DICOM format and have noticed that not all feasible gray levels are used in the representation of the pixels of the image. It has been found that generally histograms follow a sort of comb representation, in which gray levels that are high populated are adjacent to unused levels. The proposed method consists in determining the levels having a suitable frequency rate that are neighboring to a zero-frequency level, instead of performing a histogram modification before the watermarking insertion as in [2]. The advantages of the method are twofold: the algorithm is greatly simplified and the distortion introduced is very small, given that only watermarked pixels are modified.

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Nonstationary biorthogonal wavelet filters

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Nonstationary multiresolution analyses have gained a great interest in recent years. In fact, in the nonstationary framework it is possible to construct nonstationary biorthogonal bases whose approximation properties are better than those achieved in the stationary case [1], [2].

Nonstationary biorthogonal bases are associated with *nonstationary biorthogonal filters*, defined by two pairs of filter sequences - the low-pass pair $\{a_k^{(j)}\}_{k \in \mathbb{Z}}$, $\{\tilde{a}_k^{(j)}\}_{k \in \mathbb{Z}}$, and the high-pass pair $\{b_k^{(j)}\}_{k \in \mathbb{Z}}$, $\{\tilde{b}_k^{(j)}\}_{k \in \mathbb{Z}}$, $j \in \mathbb{N}$ - whose taps change at each step j of the decomposition/reconstruction scheme, while satisfying the *biorthogonality relations*

$$\begin{aligned} \sum_k a_k^{(j)} \tilde{a}_{k-2\ell}^{(j)} &= 2\delta_{0\ell}, & \sum_k b_k^{(j)} \tilde{b}_{k-2\ell}^{(j)} &= 2\delta_{0\ell}, & \ell \in \mathbb{Z}, j \in \mathbb{N}. \\ \sum_k a_k^{(j)} \tilde{b}_{k-2\ell}^{(j)} &= \sum_k b_k^{(j)} \tilde{a}_{k-2\ell}^{(j)} = 0, \end{aligned}$$

Nonstationary filters can be used to realize *nonstationary wavelet transforms* through a classical *subband coding* (analysis/synthesis) scheme, which permits to change the properties of the analysis/synthesis filters at each decomposition/reconstruction level. This property makes them a flexible and adaptive tool to be successfully applied in signal and image processing, while preserving all the computational advantages of the discrete wavelet transform.

In this work we will present some families of nonstationary biorthogonal wavelet filters and analyze their main properties - compact support, number of vanishing moments, regularity, etc. - that contribute to the good compaction property of the nonstationary wavelet transform in both time and frequency domains. The performances of such filters in some classical problems, such as compression, denoising and edge detection, will be also evaluated.

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Synthesis of coloured maps from keratography

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The map with coloured strips that is output of the computer connected to the keratographer shows the curvature of the cornea; it allows to put in evidence anomalies such as the keratoconus and it is useful when planning a refractive surgical operation and when monitorating the healing afterwards [1].

We have studied how to describe a map in a concise way such that $4 * 10^3$ bytes are enough to store the important information.

We recover the map on the basis of the compressed information: the fast algorithm makes use of the structure 'contour tree' for the correct assignment of the colour.

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Partition of unity algorithms for two-dimensional interpolation using radial basis functions

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In this contribution we present fast algorithms to be used in applications of two-dimensional interpolation processes. These procedures are characterized by the use of efficiently implemented searching techniques, which exploit a suitable and optimal partition of the domain in a number of strips. The interpolation schemes are based on partition of unity methods, which make use of radial basis functions as local approximants. Numerical experiments show accuracy of the considered methods and efficiency of the related algorithms. Finally, applications to Earth's topography are considered.

Medical image registration using compactly supported functions

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In this contribution we consider landmark-based image registration using radial basis function interpolation schemes. More precisely, we analyze some landmark-based image transformations using compactly supported radial basis functions, namely multivariate Wendland's functions and products of univariate Wendland's functions. Comparisons with other interpolation techniques are performed. Numerical experiments show accuracy and stability in some test cases of the considered approaches and also their applicability to real medical images.

Reconstruction of volume data by trivariate quartic C^2 box splines

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The construction of non-discrete models from given discrete data on volumetric grids and isosurface extraction [2] is an important problem in many applications, such as scientific visualization, computer graphics and medical imaging. In fact the volume data sets typically represent some kind of density acquired by devices like CT or MRI sensors. Such type of input data is structured so that the samples are arranged on a regular three-dimensional grid. In order to process these gridded samples an appropriate non-discrete model is required.

Beside classical discrete models, in literature non-discrete ones based on 3D tensor product splines, blending sums of univariate and bivariate splines, trivariate quadratic and cubic C^1 splines given in Bernstein-Bézier form and quintic C^2 box splines are proposed ([1,3,4,5] and references therein).

In this work we develop spline methods, based on trivariate quartic C^2 box splines on type-6 tetrahedral partitions, which can be used for an efficient reconstruction and visualization of gridded volume data.

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CAD system for the treatment of neurological bioimages

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Computer-Aided Diagnosis (CAD) has become one of the major research subjects in medical imaging and diagnostic radiology. It provides two main actions: image analysis and identification of ROI. The CAD phases are: Pre-processing; Processing and Segmentation; Features Extraction and Classification [1]. In this paper, a CAD system has been developed to assist radiologists in the evaluation of Computed Tomography (CT) and Magnetic Resonance Imaging (MRI) of Alzheimer Disease (AD) and Multiple Sclerosis (MS) patients. Images have provided by IRCCS Centro Neurolesi Bonino-Pulejo of Messina, in their original format. The MS project allow a clear classification of image characteristics of different regions (lesions and no-lesions) within the same image MRI. For the phase of detection and extraction of lesions in the images, we applied the Watershed segmentation. To overcome the problem of over-segmentation we used a Cluster Analysis to classify image features as lesion and no-lesion [2]. The AD project aims to generate a model, based on Active Appearance Model (AAM), for brain matter and ventricular area classification and segmentation and to evaluate quantitative and volumetric variation of the two regions of patients with AD, over time in CT images. We aim to find, a correlation between the changes in cerebral mass and the results obtained through traditional tests for the evaluation of cognitive deficits (eg MMSE) [3]. Such a CAD system could, therefore, support the activities to clinical interpretation of images of MS and AD, resulting from this system a second opinion.

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3. Cootes, T.F. and Edwards, G.J. and Taylor C.J. 1998 Active Appearance Models. In *European Conference on Computer Vision* (ed. H.Burkhardt and B. Neumann), vol. 2, pp. 484498. Springer.

MSP 06-08 - Complex systems

I - II - III

Collective behavior of a nonlinear system does not correspond to the dynamics of its components. The interaction between parts of the system determine unexpected behaviors in many instances. Complex systems approach focus on the effects on the global dynamics of the interactions between the parts of the system. Often the collective dynamics features are hidden when one studies the single components properties. Furthermore an oversimplification of the components dynamics may destroy the emergence of specific collective dynamics.

Complex system structure arises in variety of fields, ranging from physics to neurosciences, ecology, social sciences, reliability theory and many other contexts. In the complex system approach different applications share the same mathematical tools. Some talks of these minisymposia analyze a specific application and describe the arising of unexpected collective behaviors. The application of specific mathematical methods to the study of crowd dynamics, vehicular traffic, reliability theory or epidemiology are some of the topics of different contributions. Despite the specificity of the discussed application, often the complex system approach used in a specific frame, may be extended to models in other contexts. This fact determines a further reason of interest for the discussed examples.

Different mathematical methods may be applied to study complex systems. The study is performed both with deterministic and stochastic methods. The development of new mathematical tools for the analysis of complex systems is a further goal for mathematicians working on models. Some talks of the minisymposia focus on such methods and on some related statistical problem.

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Multiscale probabilistic models for collective behaviors in living complex systems - Focus on crowd dynamics

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Crowd dynamics are ruled by mutual interactions among the walkers, which continuously modify local individual walking paths. Self-organized flow patterns then emerge, that can be clearly seen at large scales. The challenging goal of the modeling approach should be devising methods able to reveal the emergence of macroscopic self-organization from the microscopic interaction dynamics. Indeed, the macroscopic information is ultimately the most useful one for quantitative purposes; on the other hand, the actual physics of crowds may not be fully caught simply by averaged approaches, because the most interesting phenomena occur out of equilibrium.

Mathematical models of crowd dynamics have been traditionally focusing on just either scale of description. In contrast, our aim is to go beyond the dichotomy microscopic/macroscopic, taking a point of view in which the two scales complement each other fruitfully. In this talk we present a measure-theoretic approach, which makes possible an Eulerian particle-free modeling of the crowd stemming from individual-based Lagrangian reasonings. In this context, we discuss the embedding of microscopic individualities into the macroscopic collective crowd flow, in cases in which the final dynamics are expected to arise from a balanced interplay between small and large scales.

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2. Cristiani, E., Piccoli, B., and Tosin, A. 2012 *How can macroscopic models reveal self-organization in traffic flow?*. Submitted (preprint available: arXiv:1203.1430).
3. Cristiani, E., Piccoli, B., and Tosin, A. 2011 *Multiscale modeling of granular flows with application to crowd dynamics*. Multiscale Model. Simul. 9, 155–182.
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5. Piccoli, B., and Tosin, A. 2011 *Time-evolving measures and macroscopic modeling of pedestrian flow*. Arch. Ration. Mech. Anal. 199, 707–738.
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Statistical study of the interaction between the spread of an influenza epidemics and human mobility

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Quantifying dissemination of infectious diseases is a key issue in their dynamics and control. In particular the regional spread of influenza epidemics has shown [3] a more close correlation with rates of movement of people to and from their workplaces (workflows) than with geographical distance.

A global structured metapopulation model integrating mobility and transportation data worldwide has been proposed in [1] and has been applied in [2] to forecast the spread of the influenza A(H1N1) pandemic in 2009. The model is based on a many-particles approach to simulate a complex system constituted by a two-layers SLIR mode. The application of this worldwide model to local realities, at the regional or national level, encounters difficulties due mainly to data availability for parameter estimation.

In this talk we present a statistical study of the relationships between the spread of the epidemics of influenza and human mobility in Northern Italy, based on data collected via the Influeweb project (<http://www.influeweb.it/>), aimed to investigate possible (robust) extensions of the models proposed in the literature to local realities, taking into account data variability.

This work is performed in collaboration with the Complex Networks Unit, directed by Dr. Vittoria Colizza at ISI Foundation, Torino, Italy.

1. Duygu Balcan, Vittoria Colizza, Bruno Goncalves, Hao Hud, Josè J. Ramasco, Alessandro Vespignani, 2009 *Multiscale mobility networks and the spatial spreading of infectious diseases*. PNAS, 106:51, 21484-21489.
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3. Cecile Viboud, Ottar N. Bjrnstad, David L. Smith, Lone Simonsen, Mark A. Miller, Bryan T. Grenfell, 2006. *Synchrony, Waves, and Spatial Hierarchies in the Spread of Influenza*. Science 312, 447–451.

A discrete kinetic theory approach to modeling vehicular traffic

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In this talk specific models for the vehicular traffic along a one-way road are presented in the framework of the Discrete Kinetic Theory Approach. Spatially homogeneous problems are studied and qualitative investigations of some cases study are discussed through the spatially inhomogeneous problems.

Improving multicomponent systems via randomization

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In reliability theory, a Parrondo's paradox involves two systems in series, the units of the first system being less reliable than those of the second. If the first system is modified so that the distributions of its new units are mixtures of the previous distributions, then under suitable conditions the new system is more reliable than the second in the usual stochastic order [1]. The lifetimes of series or parallel systems formed by nonindependent components are also considered: they may be stochastically improved by replacing the lifetimes of each component by an independent mixture of the individual components lifetimes [2].

We also show that randomization may achieve a better reliability in a multicomponent system, when the components are randomly chosen from two different batches. The system reliability increases, in usual stochastic order, as the random number of components chosen from the first batch increases in increasing convex order [3].

1. Di Crescenzo, A. 2007 *A Parrondo paradox in reliability theory*. The Mathematical Scientist 32, 17–22.
2. Di Crescenzo, A. and Pellerey, F. 2011 *Improving series and parallel systems through mixtures of duplicated dependent components*. Naval Research Logistics 58, 411–418.
3. Di Crescenzo, A. and Pellerey, F. 2011 *Stochastic comparisons of series and parallel systems with randomized independent components*. Operations Research Letters 39, 380–384.

A mathematical model for value estimation with public information and herding

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This talk deals with a class of integro-differential equations modeling the dynamics of a market where agents are called to estimate the value of a given traded good. Two basic mechanisms are assumed to concur in value estimation: interactions between agents and some sources of public information and herding phenomena. A general well-posedness result is established for the initial value problem linked to the model and the asymptotic behavior in time of the related solution is characterized for some general parameter settings, which mimic different economic scenarios. Analytical results are illustrated by means of numerical simulations and lead us to conclude that, in spite of its oversimplified nature, this model is able to reproduce some emerging behaviors proper of the system under consideration. In particular, consistently with experimental evidence, the obtained results suggest that if agents are highly confident in the product, imitative and scarcely rational behaviors may lead to an over-exponential rise of the value estimated by the market, paving the way to the formation of economic bubbles.

A statistical approach to recognize interactions between neurons

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To understand neuronal code it is important to know the structure of the neuronal network. Unfortunately the only information available on this complex structure comes from recorded spike trains. This makes necessary to develop statistical methods to guess possible connections from available data.

To this aim we assume that the membrane potential evolution is described by a Leaky integrate and fire model [2], the inter-times between successive spikes of a neuron are independent identically distributed random variables (r.v.s) T_i , $i = 1, \dots, n$ and we look for the dependencies between spike trains [1].

We propose to study the copula between the inter-times of pairs of spike trains and we test the shape of the resulting copula to detect the possible dependencies between the involved r.v.s. The method allows to recognize delayed dependencies as well as relationships between simultaneous spikes. Furthermore, it can be extended to the case of multiple spike trains.

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2. Sacerdote, L. and Giraud, M.T. *Stochastic Integrate and Fire Models: a review on mathematical methods and their applications*. LNMBios, in press.

Segregation and dynamics of reaction-diffusion systems in the presence of strong competition

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Several physical phenomena can be described by a certain number of densities (of mass, population, probability, ...) distributed in a domain and subject to phenomena of diffusion, reaction, and competitive interaction. Whenever the competitive interaction is the prevailing phenomenon, one reasonably expects that the several densities can not coexist and tend to segregate, hence determining a partition of the domain. In a series of recent works in collaboration with Conti, Verzini, Noris and Tavares, we have been interested in the analysis of the qualitative properties of solutions of systems of semilinear elliptic equations, whenever the parameter describing the competitive interaction diverges to infinity. Of course, the partition becomes the main object of investigation both from the analytical point of view than from the geometric, with emphasis on the points of multiple intersection. When the system possesses a variational structure, one can associate an optimal partition problem with the ground states. Conversely, as we did in joint papers with Helffer and Hoffmann-Ostenhof, one can regard at optimal partitions related to linear or nonlinear eigenvalues as limits of competing systems as the competition parameter diverges.

1. H. Berestycki, S. Terracini, K. Wang and J.C. Wei, *Existence and Stability of Entire Solutions of An Elliptic System Modeling Phase Separation*, preprint (2012), arXiv:1204.1038
2. L. A. Caffarelli, A. L. Karakhanyan and F. Lin, *The geometry of solutions to a segregation problem for non-divergence systems*, J. Fixed Point Theory Appl. 5 (2009), no.2, 319-351.
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4. M. Chang, C.S. Lin, T.C. Lin and W.W. Lin, *Segregated nodal domains of two-dimensional multispecies Bose-Einstein condensates*, Phys. D 196 (2004), no. 3-4, 341-361.
5. M. Conti, S. Terracini and G. Verzini, *Asymptotic estimates for the spatial segregation of competitive systems*, Adv. Math. 195(2005), no. 2, 524-560.
6. E.N. Dancer, K. Wang and Z. Zhang, *The limit equation for the Gross-Pitaevskii equations and S. Terracini's conjecture*, preprint 2011.
7. B. Helffer, T. Hoffmann-Ostenhof and S. Terracini, *Minimal partitions in dimension 3*, Discrete and Continuous Dynamical Systems A, 28 (2010), 617-635
8. B. Helffer, T. Hoffmann-Ostenhof and S. Terracini, *On Spectral Minimal Partitions: the Case of the Sphere*, in *Around the Research of Vladimir Maz'ya III. Analysis and Applications* Ari Laptev (Ed.). International Mathematical Series. Vol. 13, Springer, 2010

9. B. Noris, H. Tavares, S. Terracini, G. Verzini, *Uniform Hölder bounds for nonlinear Schrödinger systems with strong competition*, Comm. Pure Appl. Math. 63 (2010), 267–302
10. H. Tavares, S. Terracini, *Sign-changing solutions of competition-diffusion elliptic systems and optimal partition problems*, Ann. Inst.H. Poincaré Anal. Non Linéaire 29 (2012), 279-300
11. H. Tavares and S. Terracini, *Regularity of the nodal set of segregated critical configurations under a weak reflection law*, (arXiv:1002.3822), Calc. Var. PDE, to appear.

From heterogeneous vehicle–driver behaviors to first order traffic flow macroscopic models

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The approach to the modeling of vehicular traffic based on the idea that vehicles on road constitute a large living, hence complex, system generates a variety of challenging analytic and computational problems. One of the greatest difficulties of the modeling approach is the selection of the representation and modeling scale between the microscopic, individual based, scale concerning the dynamics of all driver-vehicle subsystems, and the macroscopic scale suitable to provide the time and space evolution of the macroscopic flow quantities, typically local density and mean velocity. It has been stated [1] that none of the scales is fully consistent; therefore multiscale methods need to be developed toward a deeper understanding of the system under consideration, which exhibits several features of complex systems. This talk proposes a two scale modeling approach to vehicular traffic, where macroscopic conservation equations [2] are closed by models at the microscopic scale obtained by a mathematical interpretation of drivers behaviors to local flow conditions. In particular we focus on the closure of the mass conservation equations by a phenomenological model derived by a detailed analysis at the scale of individual vehicles. The heterogeneous behavior of the driver-vehicle micro-system is taken into account.

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2. N. Bellomo and V. Coscia, First order models and closure of the mass conservation equation in the mathematical theory of vehicular traffic flow, *Comptes Rendus Mécanique*, vol. 333 (2005) pp. 843–851.

Optimal kinematics of supercoiled filaments

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In this talk new kinematics of supercoiling of closed filaments as solutions of the elastic energy minimization are proposed [2]. The analysis is based on the thin rod approximation of linear elastic theory, under conservation of self-linking number with elastic energy evaluated by means of bending and twisting contributions. The model requires a monotonic decreasing behavior in time of the elastic energy, favoring the folding process, it includes constraints to ensure the inextensibility of the filament and prescribed initial condition on critical twist value to generate writhing instability [1]. Time evolution functions are described by means of piecewise polynomial transformations based on cubic B-spline functions considering the corresponding de Boor control points as the unknowns in a non-linear optimization problem. We show how the coiling process is associated with conversion of mean twist energy into bending energy through the passage by an inflexional configuration in relation to geometric characteristics of the filament evolution. These results find useful applications in the general context of structural genomics and proteomics [3].

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3. Ricca, R. L. and Maggioni, F. 2008 *Multiple folding and packing in DNA modeling*. Comp. & Maths. with Appl. 55, 1044-1053.

A discrete model analyzing biophysical determinants of cell migration in matrix environments

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Cell migration on and through extracellular matrix plays a critical role in a wide variety of physiological and pathological phenomena, and in scaffold-based tissue engineering. Migration is regulated by a number of extracellular matrix- or cell-derived biophysical parameters, such as matrix fiber orientation, gap size, and elasticity, or cell deformation, proteolysis, and adhesion. We here present an extended Cellular Potts Model (CPM, [1,2]) able to qualitatively and quantitatively describe cell migratory phenotype on both two-dimensional substrates and within three-dimensional environments, in a close comparison with experimental evidence. As distinct features of our approach, the cells are represented by compartmentalized discrete objects, differentiated in the nucleus and in the cytosolic region, while the extracellular matrix is composed of a fibrous mesh and of a homogeneous fluid. Our model provides a strong correlation of the directionality of migration with the topological ECM distribution and, further, a biphasic dependence of migration on the matrix density, and in part adhesion, in both two-dimensional and three-dimensional settings. Moreover, we demonstrate that the directional component of cell movement is strongly correlated with the topological distribution of the ECM fibrous network. In the three-dimensional networks, we also investigate the effects of the matrix mechanical microstructure, observing that, at a given distribution of fibers, cell motility has a subtle bimodal relation with the elasticity of the scaffold. Finally, cell locomotion requires deformation of the cells nucleus and/or cell-derived proteolysis to overcome steric fibrillar obstacles within rigid matrices characterized by small pores.

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On the dynamics of social conflicts: looking for the Black Swan

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This communication focuses the modeling of social competition, possibly resulting in the onset of extreme conflicts. More precisely, we discuss models describing the interplay between individual competition for wealth distribution that, when coupled with political stances coming from support or opposition to a government, may give rise to strongly self-enhanced effects. The latter may be thought of as the early stages of massive, unpredictable events known as Black Swans, although no analysis of any fully-developed Black Swan is provided here. The approach makes use of the framework of the kinetic theory for active particles, where nonlinear interactions among subjects are modeled according to game-theoretical tools.

Mathematical tools to model the interactions in a neural network

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Neural networks are a typical example of complex system. The level of refinement of their description strongly depends upon the aims the models. Nowadays there exist good models for the description of single neuron dynamics. Mathematical tools for their analysis have been developed. Biophysical models consider the ion dynamics through the membrane while stochastic diffusion models, of Leaky Integrate and Fire type, summarize the ionic transfer in a noise term. More sophisticated models look at the membrane potential evolution as the result of further microscopic phenomena.

However the interest is now focused on neural networks. Often models make use of oversimplified descriptions of the single neuron activity to become able to simulate large networks. This fact prevents the recognition of possible effects related with the interaction of the dynamics of involved neurons. Our approach aims to cover this gap. We want to use existing Leaky Integrate and Fire models to describe neural networks and to recognize the effect of the interaction between neurons on neural code. Due to the lack of mathematical tools for this scope, we focus here on the selection of suitable mathematical tools for this study. Copulas as well as Cox Method are possible candidates.

**MSP 09-10 - Computational and statistical methods for
biomedical applications
I - II**

This minisymposium considers computational and statistical methods for biomedical applications. The complexity and high-dimensionality of the data provided by diagnostic medical devices (such as angiographies, tomographies and magnetic resonance imaging devices), and the complexity of the biological phenomena investigated, call for the development of novel advanced computational and statistical methods for a quantitative description of such phenomena. The minisymposium aims in particular at showcasing recent and innovative techniques including wavelets-based methods, strategies for the solution of the fluid-structure interaction problem in haemodynamics, methods for surface fitting with differential regularizations and for the reconstruction of three-dimensional geometries, models for shape analysis. All these techniques are presented in relation to a precise biomedical application.

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A variational approach for image-based parameter estimation in hemodynamics

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Estimation of the stiffness of a biological soft tissue is useful for the detection of pathologies such as tumors or atherosclerotic plaques. One of the methods used to estimate such parameter is called *elastography*: a known force is applied to the tissue and the corresponding deformation is stored. An inverse elasticity problem is then solved to estimate the physical parameters, such as the Young modulus. In the case of arteries, there is already a natural force applied to the vessel, given by the action of the blood. However, since this force is not known, in order to estimate the Young modulus an inverse fluid-structure interaction (IFSI) problem needs to be solved. First, we introduce a variational approach to solve this problem, together with some well posedness results. A numerical analysis of synthetic problems with and without noise is then presented. Finally, we give some preliminary results of possible research directions aiming to cut down the high computational costs of the IFSI problem.

Validation of a high-flow rate fluid solver with application to arterio-venous fistula hemodynamics

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Patient-specific computational hemodynamics has proven to be a reliable tool for estimating flow, pressure fields and wall shear stress distributions *in vivo*. However, in the specific case of arterio-venous fistula (AVF) for patients on hemodialysis therapy, the non-physiological conditions occurring after anastomosis creation, such as high blood flow rates and flow instabilities, pose a potential challenge to numerical solution strategies.

In this talk we present the validation of the incompressible Navier-Stokes (INS) finite element solver introduced by Botti and Di Pietro [1] with application to a patient specific AVF surgically created to provide a vascular access for hemodialysis. Such strategy, implemented in the open-source hemodynamics solver Gnuid [2], offers a very favorable trade-off between computational cost and robustness with respect to convection-dominated flows in complex 3D geometries, making the approach particularly suitable for hemodynamic applications in the context of patient-specific simulation in population studies.

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2. Gnuid, a dG-cG Pressure-Correction INS Solver for Hemodynamics, <https://github.com/lorbot/Gnuid>.

Numerical simulations for percutaneous vascular surgery: from diagnosis to prediction

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Cardiovascular diseases (CDVs) such as stroke, heart attacks, aortic aneurysms, are a social and economical emergency in Western countries. Current clinical trend is directed to minimize the impact of surgical procedure to reduce post-operative care and costs. Within this context, dedicated simulations can support the procedure planning and device tailoring toward patient-specific treatments. In this presentation, we firstly discuss the use of finite element analysis to investigate different mini-invasive cardiovascular procedures (from carotid stenting to endovascular aortic aneurysm repair) [1,2,3].

We will also discuss the application of a innovative computational approach, i.e., Isogeometric Analysis (IGA)[4], as a valid alternative to classic techniques based on the finite element method. In particular we focus on the complex structural behavior of the aortic valve moving from the analysis of a single leaflet closure to the study of the whole aortic anatomical region including both the leaflets, which are the most flexible parts of the valve, and the root, i.e., the surrounding vessel wall.

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High performance finite elements library LifeV: a fluid-structure interaction module for hemodynamic applications

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The increasing computational load required by most applications and the limits in hardware performances affecting scientific computing contributed in the last decades to the development of heterogeneous parallel software, protocols and architectures.

In Fluid-Structure Interaction (FSI) for haemodynamic applications, parallelization and scalability are key issues. We use a class of parallel solvers and preconditioners for the FSI problem obtained by exploiting the block-structure of the linear system. We then analyze their performance for both academic examples and physiological test cases.

We present a geometrical multiscale approach in which one dimensional models are coupled with a fully 3D FSI arterial segment, focusing on the coupling algorithm and on the numerical reflections issue. Eventually we compare different isotropic elastic structural models on a physiological test case.

Modeling mandibular shape variation using Bayesian ANOVA models

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The mandible is a moving bone, and its growth and remodeling is dependent on the growth and biomechanical forces of all other component structures (bony and soft tissue structures) in the craniofacial complex. Craniofacial development and growth involve both size and shape variations. The anthropological and clinical significance of these changes is related to the assessment of growth potentials, the diagnosis of skeletal disharmonies, and the establishment of a proper orthopedic/orthodontic treatment plan. Although the literature describes growth extensively (Enlow, 1982), growth problems related to the cranial and facial structures are of a very intricate nature and have not yet been fully clarified. For example, the amounts of growth that occur, and the sites where it is most active during different stages of development must be better understood. The purpose of this work is to quantitatively characterize the shape variation of a set of mandibles recorded in a longitudinal study. We do this by first summarizing the mandible by a continuous outline and then using a functional analysis of variance - ANOVA - model to describe the different sources of variability. The model allows for dimensionality reduction and can be used to represent the main modes of variation of the mandibles.

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PDE penalized statistical estimation of blood flow velocity profiles

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In this work we describe a novel statistical technique for the estimation of blood velocity profiles in a section of the carotid artery, using data provided by eco-color Doppler images. In particular, following the approach typical of functional data analysis, we propose a bivariate generalization of smoothing splines. The surface estimate is obtained via minimization of a penalized sum-of-square-error functional where the roughness penalty consists in the L2 norm of a second order partial differential operator. The method is thus well suited for applications where the knowledge of the problem suggests the choice of a differential operator modeling to some extent the phenomenon under study. For instance in the application of the blood velocity profile estimate, the differential operator considered is an approximation of the Navier-Stokes equations. The minimization problem defining this surface estimator is shown to have a unique solution, which is approximated by means of the finite element method. The surface estimator is linear in the observations and some classical inferential results are derived, providing uncertainty quantification for the estimate.

Interpolation-based reconstruction of human carotid dynamics from magnetic resonance images

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Knowledge of the three dimensional (3D) motion field of the carotid bifurcation is important for several applications, such as the study of the associations between atherosclerosis and mechanical properties, vessel compliance estimation or data assimilation.

A widespread non-invasive method for imaging wall motion in clinical settings is 2D-cine-MRI, whereby individual slices are acquired along the carotid bifurcation with a thickness of 3 to 6 mm, in which carotid wall motion is sampled with a temporal resolution of 20-25 frames per cardiac cycle. These data are complemented with a 3D static image (3D-MRI) of the entire vessel.

In this work, we propose a method to reconstruct the complete 3D carotid motion field starting from thick-sliced 2D-cine-MRI and static 3D-MRI data. Both 2D and 3D images are segmented using a level-set method, and lumen boundary displacements at the individual slice locations are computed. After registering 2D contours and the relative displacements to the static 3D model, the 3D deformation field is reconstructed by solving an harmonic equation on the 3D surface and interpolating displacements along the lines of steepest descent of the harmonic solution.

In addition to demonstrating results on clinical data, the method is validated by comparing the displacement field obtained through a fluid-structure interaction simulation, assumed as gold standard, and the displacements reconstructed from slices of the same displacement field, for slice thicknesses ranging from 3 to 6mm.

Mammogram diagnostics via 2-D complex wavelet-based self-similarity measures

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Breast cancer is the second leading cause of death in women in the United States. Mammography is currently the most effective method for detecting breast cancer early; however, radiological interpretation of mammogram images is a challenging task. On the other hand, many medical images demonstrate a certain degree of self-similarity over a range of scales which can help us in their description and classification. In this work, we generalize the scaling-mixing wavelet spectra to the complex wavelet domain. In this domain, we estimate Hurst parameter and phase and use them as discriminatory descriptors to classify mammographic images to benign and malignant. The proposed methodology is tested on a set of images from the University of South Florida Digital Database for Screening Mammography (DDSM).

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3. Hamilton, E. K., Jeon, S., Cobo, P. R., Lee, K. S., and Vidakovic, B. 2011. *Diagnostic classification of digital mammograms by wavelet-based spectral tools: A comparative study*. The Proceedings of the 2011 IEEE International Conference on Bioinformatics and Biomedicine, 384–389.

MSP 11-13 – Developments of graph theory to networks I - II - III

In the last years, Commutative and Combinatorial Algebra have paid particular attention to large classes of monomial ideals derived from graphs in order to describe algebraic properties of them. Such ideals turn out to be very interesting from a combinatorial point of view too. For instance, in the squarefree case, their link with simple graphs, simplicial complexes, etc. makes them precious for the application in different spheres.

The aim of the present minisymposium is to explain how algebraic and geometric 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.). The proposal covers recent developments within this ambit, checking to translate or evaluate theoretic results into concrete examples.

Classical topics include the algebraic theory of the edge ideals, namely monomial ideals generated in degree two which descend from the arcs of a graph. Further arguments regard the Groebner bases theory with the study of monomial subrings and toric ideals derived from them. By using such tools, many improvements have been achieved within the limits of these sciences.

Finally, using the notion of minimal covering for the nodes of a graph, recent results show that it is possible to attach to graphs the so-called ideals of vertex covers; an intensive study of them carries to solve interesting and unthinkable problems related to these fields.

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Ideals of vertex covers and applications

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Classes of simple graphs are studied using computational and algebraic methods in order to give geometric models of a network and of its connectivity. Let \mathcal{G} be a simple graph on n vertices v_1, \dots, v_n and $I(\mathcal{G}) \subset R = K[X_1, \dots, X_n]$, K a field, be its edge ideal. $I(\mathcal{G})$ is generated by squarefree monomials of degree two, $I(\mathcal{G}) = (\{X_i X_j \mid \{v_i, v_j\} \text{ is an edge of } \mathcal{G}\})$. The *ideal of vertex covers* of $I(\mathcal{G})$, denoted by $I_c(\mathcal{G})$, is the ideal of R generated by all monomials $X_{i_1} \cdots X_{i_k}$ such that $(X_{i_1}, \dots, X_{i_k})$ is an associated prime ideal of $I(\mathcal{G})$ ([3]).

It is examined a wide class of squarefree edge ideals associated to the connected graphs \mathcal{H} , on n vertices, consisting of the union of a complete graph K_m , $m < n$, and star graphs with centers the vertices of K_m ([1]). Some algebraic aspects linked to the minimal vertex covers for such classes of graphs can be considered. Keeping in mind the one to one correspondence between minimal vertex covers of any graph and minimal prime ideals of its edge ideal, we determine the structure of the ideal of vertex covers $I_c(\mathcal{H})$ and we study some properties. We prove that $I_c(\mathcal{H})$ has linear quotients, but in general it has not a linear resolution because it is not generated in the same degree. Using theoretic properties of the graph \mathcal{H} and algebraic properties of its edge ideal, like the Cohen-Macaulay property, we can obtain the condition such that $I_c(\mathcal{H})$ has linear resolution. Moreover, using the technique of studying the linear quotients of such ideals, standard algebraic invariants are computed ([2]).

Our aim is to study these algebraic developments of graph theory through suitable applications in real connection problems. In transport geography most networks have an obvious spatial foundation, namely road, transit and rail networks. The algebraic procedures introduced are good instruments concerned about how networks can be encoded and their properties measured.

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Node coverings in presence of loops

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In [1], [2] remarkable classes of simple graphs were introduced showing that algebraic properties and invariants of their edge ideals are retained when some loops are put in them.

Let \mathcal{G} be a graph on vertex set $V(\mathcal{G}) = \{v_1, \dots, v_n\}$ set of edges $E(\mathcal{G})$ and set of loops $L(\mathcal{G})$. The *edge ideal* $I(\mathcal{G})$ of \mathcal{G} is defined to be the ideal of the polynomial ring $R = K[X_1, \dots, X_n]$, K a field, generated by monomials $X_i X_j$ such that $\{v_i, v_j\} \in E(\mathcal{G}) \cup L(\mathcal{G})$. In [2] we examined both connected loopless graphs \mathcal{H} on n vertices, consisting of a complete graph K_m , $m < n$, together with star graphs with centers the vertices of K_m , and connected graphs with loops \mathcal{K}' , built from \mathcal{H} by adding loops on nodes of them. The *ideal of vertex covers* $I_c(\mathcal{G})$ of $I(\mathcal{G})$, first introduced in [4], represents the algebraic transposition of the concept of (minimal) vertex covering for a graph \mathcal{G} . It is defined to be the ideal of R generated by all monomials $X_{i_1} \dots X_{i_r}$ such that $(X_{i_1}, \dots, X_{i_r})$ is an associated minimal prime ideal of $I(\mathcal{G})$. When \mathcal{G} possesses loops, the structure of $I_c(\mathcal{G})$ is $(\cap_{i,j} (X_i, X_j) \mid \{v_i, v_j\} \in E(\mathcal{G}), i \neq j) \cap (X_k \mid \{v_k, v_k\} \in L(\mathcal{G}), k \neq i, j)$. Investigating the generators, we are able to highlight some algebraic aspects of $I_c(\mathcal{K}')$. In particular, we prove that there exists an ordering on the number of variables of every monomial of $I_c(\mathcal{K}')$ for which this ideal admits linear quotients and write them explicitly; we also examine subclasses of graphs \mathcal{K}' whose ideals of vertex covers are generated in the same degree, so that these ideals have linear resolution; and we compute standard algebraic invariants of $I_c(\mathcal{K}')$ too. Finally, because the ideals $I_c(\mathcal{H})$ are Cohen-Macaulay, we show that the property is preserved for the ideals $I_c(\mathcal{K}')$ related to graphs \mathcal{K}' which have loops on all the vertices corresponding at least to a monomial generator of $I_c(\mathcal{H})$. The study of such facts is devoted to find specific useful tools for improving actual critical situations for the connections in the field of communications and transport.

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Vertex cover ideals of chordal graphs

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We investigate the structure of vertex cover ideals of some classes of chordal graphs and of their powers. We are interested in homological and combinatorial properties. We also discuss on a conjecture due to Herzog, Hibi and Ohsugi ([2]) that all powers of the vertex cover ideal of a chordal graph are componentwise linear. The study of vertex cover ideals can be useful, for instance, in computer network security.

1. C. A. Francisco, A. Van Tuyl 2007 *Sequentially Cohen Macaulay edge ideals*. Proc. Amer. Math. Soc. 135, 2327-2333,
2. J. Herzog, T. Hibi, H. Ohsugi 2011 *Powers of componentwise linear ideals*. Combinatorial Aspects of Commutative Algebra and Algebraic Geometry Abel Symposia, Volume 6, 49-60.

On the h - vector of some simplicial complexes and their applications

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In this talk I will present a joint work with Naoki Terai. We characterize the h -vector of a certain class of pure and Cohen-Macaulay simplicial complexes. We consider some applications to computational geometry, to information theory, to geometric modeling and to model topology in Geographic Information Systems.

1. Bonanzinga, V. and Terai, N., 2012 *On the h -vector of pure and Cohen-Macaulay simplicial complexes associated with squarefree lexsegment ideals and some applications*, Preprint.
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5. Grandis, M., 2002, *An intrinsic homotopy theory for simplicial complexes, with applications to image analysis*, Appl. Cat. Structures 10, 99-155.
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7. Kong, T. Y. , Rosenfeld, A., 1989, *Digital Topology: Introduction and survey*, Computer Vision, Graphics and Image Processing, 48, 357-393.
8. Robins, V., 2002, *Computational Topology for Point Data: Betti Numbers of Alpha-Shapes*, pp.261-275, in Morphology of Condensed Matter: Physics and Geometry of Spatially Complex Systems, Lecture Notes in Physics 600, Springer.
9. Stanley, R., 1985, *The number of faces of simplicial polytopes and spheres*, Discrete Geometry and Convexity (J.E. Goodman et. Al., eds.), Annals of the N.Y. Acad. Sci. 440, 212-223.

Binomial ideals and graphs

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Our aim is to describe families of graphs arising from the Segre product of varieties using the theories of Gröbner basis and of affine semigroup rings.

In [1] and [2], we describe families and subfamilies of connected graphs arising from the Segre product of an r -Veronese variety and an s -Veronese variety, both square-free. In particular the kernel of the presentation of the Segre product is called Toric ideal and it is a binomial ideal. The crucial point is to study the kernel of the associated affine semigroup map π in order to obtain properties of the correspondent graph. To be precise, introduce a configuration $\mathcal{A} = \{\underline{a}_1, \dots, \underline{a}_n\} \subset \mathbb{Z}^d$ and consider the semigroup homomorphism $\pi : \mathbb{N}^n \rightarrow \mathbb{Z}^d$, $\underline{u} = (u_1, \dots, u_n) \rightarrow u_1 \underline{a}_1 + \dots + u_n \underline{a}_n$, whose image is the semigroup $\mathbb{N}\mathcal{A} = \{\lambda_1 \underline{a}_1 + \dots + \lambda_n \underline{a}_n, \lambda_i \in \mathbb{N}\}$. For each $\underline{c} \in \mathbb{Z}^d$, if \mathcal{F} is any finite subset of $\text{Ker } \pi$ it is possible to define a graph, denoted by $\pi^{-1}(\underline{c})_{\mathcal{F}}$, which has the elements of the fiber $\pi^{-1}(\underline{c})$ as vertices and two vertices \underline{u} and \underline{u}' are connected by an edge if $\underline{u} - \underline{u}' \in \mathcal{F}$ or $\underline{u}' - \underline{u} \in \mathcal{F}$ (see [4]).

Here we study the Segre product of a projective space and a square-free r -Veronese variety in order to describe families of graphs that represent real models in the networks field.

1. G.Failla, *Moves for Segre products of Veronese subrings*. Rendiconti del Circolo Matematico di Palermo, Serie II, Suppl. 80(2008), pp. 161- 167
2. G.Failla, R.Utano, *Connected graphs arising from products of Veronese varieties*. 2012 (preprint)
3. B.Sturmfels, *Gröbner bases and Convex polytopes*. Univ.Lect.Series,Vol.8, Amer.Math.Soc., 1995

Graphs arising from mixed products ideals

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Let G be a graph with vertices v_1, v_2, \dots, v_n . An algebraic object attached to G is the edge ideal $I(G)$, a monomial ideal of the polynomial ring in n variables $R = K[x_1, x_2, \dots, x_n]$, K field. Standard algebraic properties of these ideals are known ([4]). We are interesting in studying algebraic properties of the so-called generalized graph ideal, denoted by $I_q(G)$, the ideal of R generated by the square free monomials $x_{i_1}x_{i_2} \cdots x_{i_q}$ such that x_{i_j} is adjacent to $x_{i_{j+1}}$ for all $1 \leq j \leq q-1$. These ideals are related with the mixed products ideals introduced in ([3]). Let $R = K[x_1, \dots, x_n; y_1, \dots, y_m]$ be the polynomial ring in two sets of variables on a field K . Given the non negative integers k, r, s, t such that $k+r = s+t$, the mixed products ideals are the monomial ideals of R :

$$L = I_k J_r + I_s J_t,$$

where I_k (resp. J_r) is the monomial ideal of R generated by all square-free monomials of degree k (resp. r) in the variables x_1, \dots, x_n (resp. y_1, \dots, y_m). We investigate, using the theory of s -sequence, introduced in ([2]), when classes of mixed products ideals are of linear type, that is to say when the Rees algebra $\mathfrak{R}(L)$ of L is isomorphic to the symmetric algebra $Sym_R(L)$ of L . Finally, we try to model situations involving the graph theory such as paths of networks, streets using this class of special ideals.

1. La Barbiera, M. and Staglianò, P.L. *Monomial ideals of linear type*. Preprint.
2. Herzog, J. Restuccia, G. and Tang, T. 2001 *s-Sequences and symmetric algebras*. Manuscripta Math. 104, 479–501.
3. Restuccia, G. and Villarreal, R. H. 2001 *On the normality of monomial ideals of mixed products*. Communications in Algebra 29(8), 3571–3580.
4. Villarreal, R.H. 2001 *Monomial Algebras*. M. Dekker Inc., New York.

Buchberger graphs

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The Buchberger graph arises from the combinatorial nature of some algebraic objects: the monomial ideals ([1]). Since the Buchberger graph G of a monomial ideal I in three variables can be nicely embedded into the staircase diagram of I , G can be visualized in \mathbb{R}^3 and can be easily studied (connectedness, planarity, ...).

We study the Buchberger graph of classes of monomial ideals in three variables in order to find applications in different fields. In general, one uses combinatorial and geometric techniques to study data associated to phenomena, being the data a lattice points set D contained in \mathbb{N}^3 . In particular, we apply the method to study data that are very regular and to connect them by the paths of the Buchberger graph associated to a monomial ideal whose generators are constructed by the set D .

1. Miller E., Sturmfels B. *Combinatorial commutative algebra*. Graduate Texts in Mathematics, Springer Verlag, New York, 2004.

Regularity of ideals associated to planar graphs

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A graph is planar if we can locate the nodes on the plan and connect them with arcs so that these arcs intersect only in the nodes they connect. If G is a bipartite planar graph, G is embedded in the plane and identifies regions; we want to consider the polarizations of cycles that bound these regions. The procedure gives new and interesting information about new objects related to the graph, in order to apply them to security problems on the roads (paths or cycles of the graph). From an algebraic point of view, we are interested to read an algebraic invariant, the regularity of the edge ideal $I(G)$ of this class of graphs, not easy to calculate. The techniques of the theory of Groebner bases are used.

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3. Villarreal, R.H. 2001 *Monomial Algebras*. Pure Appl. Math., M. Dekker Inc., New York.

Combinatorics of planar graphs

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Planar graphs are a big class of graphs that are models for different life phenomena. Methods of combinatorial commutative algebra can be used to study their properties in terms of algebraic invariants, in order to classify phenomena.

In this work we employ techniques of Gröbner basis theory, polarization, simplicial complexes, for studying planar graphs arising from strings of integers of same length, identified with generators of monomial ideals. An application is given when the data arise from samples in statistic, also for the bipartite case (see[1]).

1. Doering L., Gunston T. *Algebras arising from bipartite planar graphs*. Comm.Algebra, Vol.24,Issue 11,1996.
2. Sturmfels B. *Groebner bases and convex polytopes* AMS University Lecture Series Vol.8,AMS,Providence,RI,1996.

MSP 014 - From nano to macro: modeling and simulation

The minisymposium deals with analytical/numerical approaches to problems which range from nano to macro geometrical scales. The first talk investigates the initial phase of multispecies biofilm development in biological fixed-growth reactors. It is described in terms of a system of nonlinear hyperbolic partial differential equations in a free boundary domain. For the first time, the dependence on substrates is here considered. A model for explaining orders of magnitude higher flow rates than what predicted by continuum fluid mechanics in a water flow through carbon nanotubes is the subject of the second talk. Its key feature lies in accounting for the work of adhesion and the surface diffusion. The third talk explores nonlocal effects in radially-symmetric heat transport inside silicon thin layers and graphene sheets. The presence of a hump in the temperature profile not allowed by the local-equilibrium theory is discussed. Finally, a problem in a macro geometrical scale is discussed: the role of the Schwarz function in two-dimensional inviscid vortex dynamics. A new equation in that function is proposed, in order to overcome the rebuilding of the Schwarz function of the boundary during the motion of a uniform vortex.

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The Schwarz function approach to the motion of planar uniform vortices

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The present talk deals with an analytical technique for approximating the dynamics of planar uniform vortices in an inviscid fluid, based on a hierarchy of linear singular integral equations. Several results will be presented for the 0-th and 1 orders solutions.

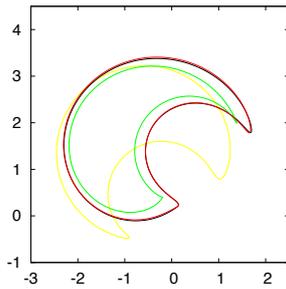
The vortex shape is accounted for at any time $t \geq 0$ through the corresponding Schwarz function, defined as $\Phi(\mathbf{x}; t) = x_1 - ix_2 = \bar{\mathbf{x}}$ in any $x_1 + ix_2 = \mathbf{x} \in \partial P(t)$. A Lagrangian approach is adopted. Named as ξ the position at $t = 0$, Φ is rewritten as $\Phi[\mathbf{x}(\xi; t); t] =: \mathbf{S}(\xi; t)$, so that for any $\xi \in \partial P(0)$: $\partial_t \mathbf{S} = \bar{\mathbf{u}}$, in which $\bar{\mathbf{u}}$ it is the conjugate velocity, related to Φ through a Cauchy integral [1]. The Laplace transform in time (indicated by a tilde) then leads to the nonlinear equation:

$$(i\sigma - 1)\tilde{\mathbf{S}}(\xi; \sigma) + \frac{1}{\pi i} \oint_{\partial P(0)} d\eta \frac{\tilde{\mathbf{S}}(\eta; \sigma)}{\eta - \xi} + \frac{1}{\pi i} \int_{\partial P(0)} d\eta \tilde{\mathbf{g}}\tilde{\mathbf{S}}(\eta, \xi; \sigma) = i\mathbf{S}_0(\xi), \quad (1)$$

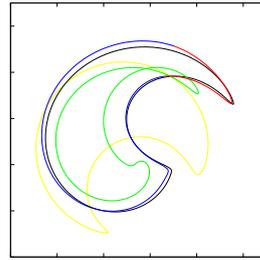
where $\mathbf{g} = \partial_\eta \log\{[\mathbf{x}(\eta; t) - \mathbf{x}(\xi; t)]/(\eta - \xi)\}$ and $\mathbf{S}_0(\xi) = \mathbf{S}(\xi; 0)$ is given. The successive approximation method is adopted to handle equation (1), by viewing the nonlinear term as a source one.

The present approach is used to investigate the dynamics of vortices, the Schwarz functions of which have two simple poles

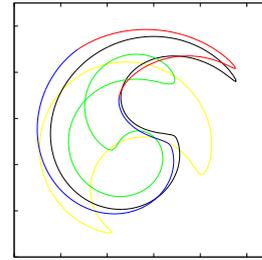
Several details about the mathematical machinery behind these solutions will be given in the talk.



(a)



(b)



(c)

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Nonlocal effects in radial heat transport in silicon thin layers and graphene sheets

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We explore nonlocal effects in radially-symmetric heat transport in silicon thin layers and in graphene sheets. In contrast to one-dimensional perturbations, which may be well described by means of the Fourier law with a suitable effective thermal conductivity, two-dimensional radial situations may exhibit a more complicated behavior, not reducible to an effective Fourier law. In particular, we show the prediction of a hump in the temperature profile for radial distances shorter than the mean-free path of heat carriers. This hump is forbidden by the local-equilibrium theory, but it is allowed in more general thermodynamic theories, and therefore it may have a special interest regarding the formulation of the second law in ballistic heat transport [1].

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DOI:10.1098/rspa.2011.0584

Analysis and simulations of the initial phase in multispecies biofilm formation

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Biofilms are widely used in wastewater treatment plants. The attachment of microbial cells to a surface represents a crucial step during start-up of a plant. Mathematical modelling of initial biofilm formation could be a useful tool to evaluate the best operational conditions maximizing the reactor performances.

In this work a mathematical modelling of the initial phase in multispecies biofilm formation is presented. Equations are derived from the mass balance for the microbial species. The biological process in one space dimension is described by the following free boundary problem

$$\frac{\partial}{\partial t} X_i(z, t) + u(z, t) \frac{\partial}{\partial z} X_i(z, t) = \rho_i r_{M,i}(z, t, \mathbf{X}, \mathbf{S}) - X_i(z, t) \frac{\partial}{\partial z} u(z, t), \quad 0 < z \leq L(t), \quad t > 0,$$

$$\frac{\partial}{\partial z} u(z, t) = \sum_{i=1}^n r_{M,i}(z, t, \mathbf{X}, \mathbf{S}), \quad 0 < z < L(t), \quad t > 0, \quad i = 1, \dots, n,$$

$$\dot{L}(t) = u(L(t), t) + \sigma, \quad t > 0,$$

$$\frac{\partial}{\partial t} S_j(z, t) - \frac{\partial}{\partial z} \left(D_j \frac{\partial}{\partial z} S_j(z, t) \right) = r_{S,j}(z, t, \mathbf{X}, \mathbf{S}), \quad 0 < z < L(t), \quad t > 0, \quad j = 1, \dots, m.$$

In above equations, $f_i(z, t)$ is the volume fraction of the microbial species i , $\sum_{i=1}^n f_i = 1$, ρ_i constant density, $X_i = \rho_i f_i(z, t)$ concentration of the microorganism i , $\mathbf{X} = (X_1, \dots, X_n)$, $S_j(z, t)$ concentration of substrate j , $\mathbf{S} = (S_1, \dots, S_m)$, $r_{M,i}(z, t, \mathbf{X}, \mathbf{S})$ specific growth rate of microorganisms, $r_{S,j}(z, t, \mathbf{X}, \mathbf{S})$ conversion rate of substrates, $u(z, t)$ velocity of the microbial mass, $L(t)$ biofilm thickness. In addition, σ denotes the biomass flux between bulk liquid and biofilm; in the most general situation, $\sigma = \sigma_{at}(t) - \sigma_{de}(L, t)$.

Under suitable hypotheses, properties of solution are investigated. Furthermore, numerical simulations are developed to evaluate the biofilm thickness, microbial species and substrate concentrations.

The results show that the attachment of microbial cells is influenced firstly by biomass flux from bulk liquid to biofilm and successively by substrate concentrations.

A mathematical model explaining high flow rate in nanotubes

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Experimental and simulation measurements of water flow through carbon nanotubes have shown orders of magnitude higher flow rates than what predicted using continuum fluid mechanics models [1-2]. A model where the effect of the work of adhesion and surface diffusion is made explicit via the Navier boundary condition of the Haagen-Poiseuille equation is proposed. The comparison between expected flows and the available experimental results shows that this model accurately predicts the flow enhancement of water in carbon nanotubes of different sizes, wall surface chemistry and structure [3].

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2. Mattia, D. and Gogotsi, Y. 2008 *Review: static and dynamic behavior of liquids inside carbon nanotubes*. Microfluid Nanofluid 5(3):289-305. doi:10.1007/s10404-008-0293-5
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**MSP 15-18 - Integral equations: numerical methods and
applications
I - II - III -IV**

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 they 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 element or finite difference methods.

Talks on theoretical contributions and/or recent applications are highly welcome.

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Gaussian rules w.r.t. exponential weights in finite or infinite intervals

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The numerical quadrature is crucial in the numerical treatment of integral equations, in particular in the Nyström methods. In this talk we consider Fredholm integral equations with kernel and/or right-hand side increasing or decreasing exponentially for $x \rightarrow \infty$. In such case the classic quadrature formulas give weak results on a theoretical and computational point of view. We propose a solution which can be used in multiple contexts.

Numerical methods for the solution of integral equations in imaging

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Many inverse problems in imaging arise from the discretization of a first kind Fredholm integral equation. The discretization process leads to an ill conditioned linear system which is usually solved by means of regularization methods. A common approach consists in the solution of a minimization problem of the form:

$$\min J(\mathbf{f}) = \|\mathbf{K}\mathbf{f} - \mathbf{g}\|^2 + \lambda(\mathcal{R}(\mathbf{f}) - \gamma) \quad (1)$$

where $R(f)$ is the regularization function, λ is the regularization parameter and γ represents the smoothness level required in the solution [1]. The function $\mathcal{R}(\mathbf{f})$ describes the kind of regularity required on the solution and its choice usually depends on the characteristics both of the image and application considered. Finding good values of λ and γ is a challenging in this framework. When white noise is added to the data, an optimal value of λ cannot be found without knowing the variance of the noise (Bakushinski's Theorem [2]). However, in imaging applications the variance of the noise is usually unknown; moreover, it is sufficient to have a good approximation of the optimal value of the regularization parameter. For this reason, different heuristic rules have been proposed in literature to compute a suitable value of λ in inverse imaging applications with unknown variance of the noise for different regularization functions $\mathcal{R}(\mathbf{f})$. We propose an iterative method [3] that finds a regularized solution \mathbf{f} computing a suitable value of λ and γ . The numerical tests performed in image denoising, deblurring and tomographic reconstruction show that the iterative method proposed is computationally efficient for large size problems. The method can be extended to more general nonquadratic objective functions, where the fit-to-function could be, for example, the Kullback-Leibler (or Csiszàr I-divergence).

1. A. N. Tikhonov, V. Y. Arsenin, *Solutions of Ill-Posed Problems*, John Wiley & Sons, 1977
2. H. W. Engl and M. Hanke and A. Neubauer *Regularization of Inverse Problems* Kluwer Academic Publishers, 1996
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A time-dependent absorbing boundary condition for the numerical solution of exterior wave equation problems

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Infinite or unbounded domains are often encountered in mathematical models associated to acoustic, aerodynamic, geophysical, electromagnetic problems; various numerical methods have been developed for them (for a survey on this topic see [1]). We consider the 2D wave equation defined in an homogeneous domain Ω^e , external to a bounded domain, and we propose a numerical scheme based on the coupling of a finite element (or a finite difference) and a boundary element method. The scheme consists of introducing an artificial boundary \mathcal{B} that determines a computational finite domain Ω , bounded internally by $\Gamma := \partial\Omega^e$ and externally by \mathcal{B} , and in using an integral relation between the solution of the differential problem and its normal derivative on \mathcal{B} . Such a relation describes a non reflecting boundary condition, non local both in space and in time. We discretize the artificial boundary condition by using a convolution quadrature formula in time (Lubich [2]) and a collocation method in space, and we use a finite element (or a finite difference) method for solving the problem associated to the bounded domain Ω .

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2. Lubich, C. 1988 Convolution quadrature and discretized operational calculus, *Num. Math.*, V. 52, pp.129145

A numerical method for the Dirichlet problem on domains with corners

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This talk deals with the numerical solution of the interior Dirichlet problem for Laplace's equation on planar domains with corners. The Authors propose a numerical method of Nyström type, based on a Lobatto quadrature rule, in order to approximate the solution of the corresponding double layer boundary integral equation. The convergence and stability of the method are proved and some numerical tests are shown.

Structured matrix spectral analysis of photonic crystals

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In this talk we illustrate both a finite difference frequency domain (FDFD) method [1] and a finite element frequency domain (FEFD) method [2] to compute the band spectra of 2D photonic crystals without impurities. Exploiting periodicity to identify discretization points differing by a period, the computational complexity of the algorithms is reduced significantly. Some preliminary considerations on the extension of the FDFD method to the 3D case are also presented.

1. Pietro Contu, C. van der Mee, and Sebastiano Seatzu *Fast and Effective Finite Difference Method for 2D Photonic Crystals*, Communications in Applied and Industrial Mathematics (CAIM), (2011); doi: 10.1685/journal.caim.374
2. Pietro Contu, C. van der Mee, and Sebastiano Seatzu. *A Finite Element Frequency Domain method for 2D Photonic Crystals*, Journal of Computational and Applied Mathematics (JCAM), (2012);doi: 10.1016/j.cam.2012.02.041

Full vectorial finite element method for integrated optical device design

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Over the last decades, the request of larger bandwidth and faster communication has strongly pushed the photonics technology. Among the several components required in photonic integrated circuits, straight waveguides and small footprint ring resonators play a key role for many applications and require sophisticated electromagnetic analysis and design.

In this work, we have studied and implemented a full vectorial modal analysis based on the finite element method for lossless waveguides and ring resonators, using cartesian and cylindrical coordinate systems, respectively. After having computed the Rayleigh-Ritz functional for the non-self-adjoint case, a fully real formulation has been derived considering isotropic, anisotropic and magneto-optical materials. Using the node-based approach, the penalty function has been introduced to remove the spurious solutions [1]. Although its use is well-known for waveguides analysis, it has been introduced for the first time in ring resonator case. Finally, the γ -formulation, where the frequency is provided as input parameter and the propagation constant is the output eigenvalue, has been derived and effectively implemented avoiding the time-consuming iterations necessary in previous formulations [2].

1. Rahman, B. M. A. and Davies, J. B. *Penalty function improvement of waveguides solution by finite elements*, IEEE Transactions on Microwave Theory and Techniques, vol. 32, pp. 922–928, August 1984.
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Parallel implementation of a SGBEM for the analysis of elastostatics 3D crack problems with unilateral contact on GPU's and multicore CPU's

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Linear Elastic Fracture Mechanics is based on the assumption, among others, that there is no contact between crack faces, resulting in the possibility of both crack opening and overclosure. While this assumption is reasonable for a significant number of crack and load configurations, it could lead to non-physical solutions in general cases, especially for mixed mode loading.

Frictionless unilateral contact between crack faces can be formulated as a Signorini-problem [2], resulting in a variational inequality which can be effectively discretized by the *Symmetric Galerkin Boundary Element Method* (SGBEM) [1]. In this context the main advantage of the symmetric formulation is that the underlying symmetry and sign-definiteness properties of the variational problem are retained in the discretization; however the need for a double integration over the crack surface of the singular kernels (which requires a $4D$ quadrature with a high number of integration points over element pairs) results in an increased computational effort.

The purpose of the present talk is to present and discuss different parallel implementation strategies with reference to modern GPU and many-core CPU architectures.

1. Bonnet, M., Maier, G., and Polizzotto, C., 1998. *Symmetric galerkin boundary element methods*. Applied Mechanics Reviews 51 (11), 669–704.
2. Kikuchi, N., Oden, J. T., 1988. *Contact Problems in Elasticity: A Study of Variational Inequalities and Finite Element Methods*. Studies in Applied and Numerical Mathematics. SIAM.

Recent advances in fracture mechanics modeling via boundary elements

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An accurate understanding of fracture initiation and propagation in different materials and at different observation scales is fundamental from the serviceability and safety standpoints of structures. The fracturing process reveals three distinct phases: loading without crack growth (steady state or stationary cracks), stable crack growth, and unstable crack growth. The problems of *crack propagation in linear elastic materials* and of *steady state cohesive-crack interfaces* will be considered in this note.

The crack propagation problem has been studied in exploiting its analogy with plasticity theory. A maximum principle was stated, that expressed the maximum dissipation at the crack tip during propagation. As a consequence, a minimum variational formulation is obtained in terms of crack tip velocity, it reminds to Ceradini's theorem for plasticity. Stability of crack path is discussed as well. Accurate evaluation of SIFs and Tstress is achieved by means of boundary integral equation. Actual features and future developments are presented.

Boundary integral equations are very attractive for steady state cohesive-crack interface problems, because all non linearities are localized on the boundary of assumed linear elastic domains. The integral operator that governs the problem is proved to be linear with respect to the rate unknown fields and symmetric with respect to a usual bilinear form in the presence of a holonomic interface law. The numerical solution of the incremental problem is then achievable by the symmetric Galerkin boundary element method.

Direct methods for CSIE in weighted Zygmund spaces with uniform norm

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This talk deals with the numerical treatment of CSIEs having compact perturbations. We propose two projection methods for solving them in the different cases where the kernels are smooth or weakly singular. Their stability and convergence are proved in Zygmund spaces equipped with uniform norm. The given error estimates cover all the ones available in literature. Some numerical examples illustrating the accuracy of the methods are shown.

Numerical analysis of nonlinear Volterra integral equations: stability with respect to bounded perturbations

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We analyze the stability properties of the solution of nonlinear Volterra integral equations of Hammerstein type:

$$y(t) = g(t) + \int_0^t k(t, s) f(s, y(s)) ds, \quad t \geq 0, \quad (1)$$

and of the numerical solution obtained by a Direct Quadrature method:

$$y_n = g_n + h \sum_{j=0}^n w_{nj} k_{nj} f(y_j), \quad n = n_0, n_0 + 1, \dots, n_0 \geq 0. \quad (2)$$

Thanks to a formal expression of the error, obtained through the resolvent kernel of its linearized equation, we provide sufficient conditions on the functions involved in (1), on the weights w_j in (2) and on the step-size h , for (1) and (2) to have the same asymptotic behavior with respect to classes of bounded perturbations. We relate our analysis to the existing theory (mainly known in the convolution case) and we give some numerical illustrative examples.

A class of methods for Volterra integral equations with periodic solution based on exponential fitting

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The mathematical modeling of some periodic phenomena with memory leads to Volterra Integral Equation with periodic solution

$$\begin{aligned} y(x) &= f(x) + \int_{-\infty}^x k(x-s)y(s)ds, & x \in [0, X] \\ y(x) &= \psi(x), & -\infty < x \leq 0, \end{aligned} \quad (1)$$

with f periodic function. Some examples are the spread of an epidemic with periodic rate of infection and feedback systems with periodic input. An accurate and efficient numerical solution of (1) requires special-purpose methods. Following the approach recently proposed in [1], and with the aim of constructing higher order methods, we formulate Direct Quadrature (DQ) methods, based on exponential fitting gaussian quadrature rules. As a matter of fact, exponential fitting is a procedure that allows to derive methods based on special functions particularly tuned to the problem [2]: in this case exponential and trigonometric functions. In the present talk, we illustrate the construction of these methods, analyze their convergence properties and make comparisons with classical DQ methods.

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An energetic approach to BEM-FEM coupling for wave propagation phenomena

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Starting from a recently developed energetic space-time weak formulation of Boundary Integral Equations (BIEs) related to wave propagation problems defined on single and multi domains [1, 2, 3, 4, 5], a coupling algorithm is presented, which allows a flexible use of finite and boundary element methods (FEM-BEM) as local discretization techniques, in order to efficiently treat interior and exterior multilayered media. Partial differential equations associated to BIEs will be weakly reformulated by the energetic approach and a particular emphasis will be given to theoretical and experimental analysis of the stability of the proposed method. First numerical results on simple wave propagation model problems will be presented and discussed.

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3. Aimi A., Diligenti M. and Panizzi S. 2010 *Energetic Galerkin BEM for wave propagation Neumann exterior problems*. CMES 58, 185-219.
4. Aimi A., Diligenti M. and Guardasoni C. 2011 *On the energetic Galerkin boundary element method applied to interior wave propagation problems*. J. Comp. Appl. Math. 235, 1746-1754.
5. Aimi A., Gazzola S. and Guardasoni C. 2012 *Energetic BEM analysis of wave propagation in 2D multilayered media*. Math. Methods Appl. Sciences, in press, DOI: 10.1002/mma.1612

Numerical modelling for EM-fields and biosystems interactions

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In this paper the electromagnetic fields related to the current sources in the human brain are investigated by means of the quasi-stationary approximation. The knowledge of these fields are of great interest to understand the human brain activity regions. By considering the current density produced by neural activity and because no current could flow out of the skull, the numerical model describing the problem can be fully defined. The current sources are simulated as current dipoles into an homogeneous sphere proceeding in the computation by solving the Poisson's equation with Neumann boundary conditions. Numerical results relating to a spherical head representation are proposed by considering also layered model with different conductivities and compared with the analytical solutions.

A stable energetic Galerkin BEM for 3D wave propagation interior problems

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Time-dependent problems, modeled by hyperbolic partial differential equations, can be reformulated by “retarded” boundary integral equations (BIEs), employing the time-domain representation formula in terms of single layer and double layer potentials. At discretization stage, usual Boundary Element Methods (BEMs) include the collocation technique with explicit evaluation of the time-convolution which is very appealing thanks to its simplicity and little demand in terms of computing effort, but always plagued with limited robustness upon variation of the time step adopted in the analysis. Improvements seems necessary, e.g. in staggered iterative coupling procedure between BEM and FEM, since stability and accuracy of the two approaches impose requirements which may be contradictory. In the talk, we focus on the three dimensional extension of the recently introduced [1] energetic Galerkin BEM for wave propagation analysis, with the aim of testing its stability and accuracy properties [2]. These are shown by means of several numerical results in case of interior problems that represent a severe test, since continuous reflection of waves in a bounded domain often gives rise, at the discretization level, to significant noise and instabilities, as stated in a huge number of literature papers.

1. Aimi A., Diligenti M. and Guardasoni C. 2011 *On the energetic Galerkin boundary element method applied to interior wave propagation problems*. J. Comp. Appl. Math. 235, 1746-1754.
2. Aimi A., Diligenti M., Frangi A. and Guardasoni C. 2012 *A stable 3D energetic Galerkin approach for wave propagation interior problems*. Submitted to Eng. Anal. Bound. Elem.

Canonical properties of general linear methods for Hamiltonian problems

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This talk is devoted to the investigation of the canonical properties of general linear methods for long time integration of Hamiltonian problems. Runge-Kutta methods exhibit some fundamental canonical properties if they are symplectic. It is known that general linear methods cannot be symplectic (see [3]), however it is possible to inherit from their nonlinear stability properties a nearly canonical behavior, known as *G-symplecticity* [1,2], which is the first ingredient to obtain an accurate conservation of the invariants of an Hamiltonian problem. Due to their multivalued nature, general linear methods generate a parasitic behavior of the numerical solution which needs to be properly removed: we discuss how G-symplectic general linear methods free from parasitism can be developed. The third aspect we aim to discuss is symmetry: in particular, we explain how time reversal symmetry allows to derive methods of a certain order by applying a reduced number of order conditions. Numerical experiments on a selection of Hamiltonian problems are discussed.

1. J. C. Butcher 2008 *Numerical methods for Ordinary Differential Equations*, Second Edition, Wiley.
2. J. C. Butcher, R. D'Ambrosio, *Partitioned general linear methods for separable Hamiltonian problems*, in preparation.
3. J. C. Butcher and L. L. Hewitt 2009 *The existence of symplectic general linear methods*, Numer. Algor. 51, 77-84.

MSP 019 - Large-scale numerical linear algebra and optimization

Numerical linear algebra and optimization are closely related and complementary. Their interplay is getting stronger and stronger, especially in the case of large-scale problems. The solution of large linear systems is a fundamental phase of many optimization methods whose success depends on the availability of effective linear algebra techniques. On the other hand, the need of solving optimization problems of increasing complexity provides new theoretical and computational challenges in numerical linear algebra. The aim of this minisymposium is to present recent advances in large-scale numerical linear algebra and their impact on optimization. The focus is on preconditioning techniques for sparse linear systems arising in interior point, Newton-like and regularization methods, as well as on recent multilevel approaches arising from the discretization of infinite-dimensional problems. Computational issues concerning the implementation on modern high-performance architectures are also discussed.

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**Quasi Newton updates of preconditioners
for large size nonlinear systems
arising in Finite Element discretizations
of groundwater flow models**

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Preconditioners for the Krylov subspace methods are studied to solve the sequence of large linearized Newton systems arising from the Richards equation as well as from multiphase flow in porous media [2,4]. Starting from a given approximation of the inverse of the initial Jacobian, such as an ILU factorization or a sparse approximate inverse (AINV), we construct a sequence of preconditioners by means of a low rank update. We prove that the constructed preconditioned matrices are not far away from the identity matrix in the Frobenius norm provided that a sufficiently good initial guess and initial Jacobian inverse approximation are provided [1,3]. Numerical results onto realistic test problems show that the low-rank modification always produce acceleration of iterative methods as compared to ILU/AINV preconditioning at every nonlinear iteration. The improvement is particularly effective in presence of ill-conditioned Jacobian matrices.

1. L. BERGAMASCHI, R. BRU, AND A. MARTÍNEZ, *Low-rank update of preconditioners for the inexact Newton method with SPD jacobian*, Mathematical and Computer Modelling, 54 (2011), pp. 1863–1873.
2. L. BERGAMASCHI, R. BRU, A. MARTÍNEZ, J. MAS, AND M. PUTTI. *Low-rank update of preconditioners for the nonlinear Richard's equation*. Mathematical and Computer Modelling. Published online on January 24, 2012:
3. L. BERGAMASCHI, R. BRU, A. MARTÍNEZ, AND M. PUTTI, *Quasi-Newton preconditioners for the inexact Newton method*, Electronic Trans. Num. Anal., 23 (2006), pp. 76–87.
4. L. BERGAMASCHI, R. BRU, A. MARTÍNEZ, AND M. PUTTI, *Quasi-Newton acceleration of ILU preconditioners for nonlinear two-phase flow equations in porous media*, Advances in Engineering Software, 46(1) (2012), pp. 63–68.

Sparse approximate inverse updated preconditioners revisited

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The search for efficient preconditioners in factorized form for Krylov subspace methods is a theme underlying the numerical linear algebra research over the last decades. Recent developments, esp. in computing hardware, have renewed the interest in updates for *approximate inverse* preconditioners for large and sparse linear systems (see, e.g., references in [1,3]), because this can mitigate very much the high computational cost required for forming the underlying factors. We will discuss some issues and show some runs for the approximate inverse preconditioners proposed by Benzi et al. and the sparsification and inversion proposed by van Duin in 1999, alternative ways of computing an approximate inverse, outlining computational costs and some other issues on conventional and innovative computing architectures like multicore CPUs and GPUs mainly in view of their use in the updating paradigm proposed in [1–3].

1. Bellavia, S. and Bertaccini, D. and Morini B. 2011 *Nonsymmetric preconditioner updates in Newton-Krylov methods for nonlinear systems*. SIAM J. Sci. Comput. 33-5, 2595–2619.
2. Benzi, M. and Bertaccini, D. 2003 *Approximate inverse preconditioning for shifted linear systems*. BIT 43-2, 231–244.
3. Bertaccini, D. and Sgallari, F. 2010 *Updating preconditioners for nonlinear deblurring and denoising image restoration*, Appl. Num. Math. 60, 994–1006.

A preconditioning framework for sequences of linear systems in optimization

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We address the problem of building preconditioners for sequences of linear systems of the form

$$(A + \Delta_k)x_k = b_k, \quad k = 1, 2, \dots,$$

where $A \in \mathfrak{R}^{n \times n}$ is symmetric positive semidefinite and sparse, $\Delta_k \in \mathfrak{R}^{n \times n}$ is diagonal positive semidefinite and the systems are compatible. Such sequences arise in many optimization methods, e.g., in affine-scaling methods for convex bound-constrained quadratic programming and bound-constrained linear least squares, and in trust-region and over-estimation methods for unconstrained nonlinear least squares. We propose a framework for building preconditioners through updates of any symmetric positive definite preconditioner for A factorized as LDL^T . The updates are low cost and preserve the sparsity pattern of L . The resulting preconditioners are effective on slowly varying sequences; furthermore, by satisfying an additional property, they get the ability of clustering eigenvalues of the preconditioned matrix when Δ_k has sufficiently large entries. We present two preconditioners in this framework, one of which extends the preconditioner in [1]. Their efficiency is confirmed by the results obtained on sequences of linear systems arising in the solution of bound-constrained convex quadratic programming problems with the reflective Newton method, and in the solution of nonlinear least-squares problems with the Regularized Euclidean Residual method.

1. Bellavia, S., De Simone, V., di Serafino D. and Morini, B. 2011 *Efficient preconditioner updates for shifted linear systems*. SIAM J. Sci. Comput. 33, 1785-1809.

Innovative multilevel techniques for structural optimization

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We address the structural optimization problem of sizing an aircraft fuselage. The problem consists in computing the dimensions of the different elements constituting a fuselage minimizing the total mass subject to some mechanical constraints. Mathematically, the problem may be formulated as a very large nonlinear optimization problem subjected to several nonlinear inequality constraints. We show that this problem possesses a natural hierarchical structure that can be exploited by a multilevel approach. This approach is innovative in the industrial sector and represents a promising alternative to the commonly employed decomposition strategies. Hence, we propose a multilevel procedure which embeds the Recursive Multilevel Trust Region method [1] into an Augmented Lagrangian framework. Some results on both academic and industrial test cases are presented.

1. Gratton, S. Mouffe, M. Toint, Ph. L. and Weber-Mendonça M. 2008 *A recursive trust-region method in infinity norm for bound-constrained nonlinear optimization*, IMA J. Numer. Anal., 28(4), 827–861.

MSP 20 - Mathematical and numerical modelling in geosciences

The use of mathematical and numerical modelling is nowadays of great importance in the field of Geosciences: many advancement of knowledge in this field heavily depends on modeling and numerical simulation. From the applicative point of view the simulation tools in geosciences are used for example in:

- industrial applications in particular in petroleum engineering;
- volcanic hazard assessment;
- earthquake forecasting;
- modelling storage of CO₂.

This minisymposium aims at collecting contribution of researchers working in the field of mathematical and numerical methods for geoscience applications. In particular the fields of mathematical geology, geophysics, basin dynamics, geodynamics and porous media flow will be considered.

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Data assimilation in distributed catchment models

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Data assimilation has received growing interest by the hydrological community due to its capability to merge observations into model prediction. We study the behavior of DA when applied to a catchment simulator coupling a three-dimensional FE Richards equation solver with a DEM based FD diffusion wave approximation for surface dynamics. Two classical approaches are compared: the Ensemble Kalman Filter and the Particle Filter. Both methods use Monte Carlo to approximate the state probability distribution by a finite number of independent model realizations, but differ in how the filtering pdf is evaluated. EnKF implements the classical Kalman filter, optimal only for linear dynamics and Gaussian error statistics. PF uses a sequential Bayesian framework and approximates the posterior probability distributions by means of appropriate weights associated to the realizations. Realizations with small weights are discarded and the Sequential Importance Resampling technique is used to maintain ensemble size. We report on the retrieval performance of the two schemes using a three-dimensional synthetic case in which multi-source observations are assimilated. The results show that EnKF Gaussian Approximation limits the accuracy and efficiency of the filter, while PF, making no assumptions on the form of the pdfs, become often more competitive.

Numerical methods for multiphase flows in fractured porous media

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Fractures can influence subsurface flows at a variety of space scales. We focus our attention on large fractures and faults which can play an important role in problems such as groundwater contamination, CO₂ storage or oil migration, acting as barriers or conduits for the flow. We employ a method based on the reduction of the fractures to 2D interfaces immersed in a 3D domain as proposed in [2]. This choice is motivated by fact that, at basin scale, the width of fractures and faults is very small compared to the typical mesh size. We allow the 2D interfaces to be non-matching with the computational grid resorting to an XFEM approximation to represent discontinuities across the fractures. The approach presented in [1] to couple, in this framework, the flow in the fracture and in the surrounding porous media has been successfully extended to the problems of passive transport in porous media, two-phase flow and to the relevant case of networks of fractures.

1. Carlo D'Angelo and Anna Scotti 2011 A Mixed Finite Element Method for Darcy Flow in Fractured Porous Media with Non-Matching Grids. In *Mathematical Modelling and Numerical Analysis*
2. Vincent Martin and Jérôme Jaffré and Jean E. Roberts 2005 Modeling fractures and barriers as interfaces for flow in porous media. In *SIAM J. Sci. Comput.*, vol. 26, pp. 1667–1691.

Asymmetry of thermal structure at slow-spreading ridges: plate kinematics, geodynamic and numerical modelling

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Plate kinematics and tectonic evolution along midocean ridges is commonly considered symmetric, when modeling with relative plate motions and steady-state processes. However, based on geological and geophysical data, some asymmetries can be observed at spreading centers. A better way to understand dynamics of lithosphere/mantle interactions and thermal structure along mid-ocean ridges, corresponds to absolute plate kinematic analyses, i.e., with respect to the mantle, modelling time-dependent tectonic processes. We performed numerical simulations of plate-driven mantle flow beneath slow-spreading ridges, and we considered a time-dependent flow induced by absolute motion of overlying rigid plates in an incompressible viscous mantle. This implies that plates along a ridge, and the ridge itself, move together with different velocities, relative to the fixed mantle, and the separation between plates triggers mantle upwelling. Numerical solutions for viscosity flow beneath plates that thicken with increasing age are presented. The mantle can be modeled as a viscous fluid, and its dynamics can be described using the Stokes equations, also including thermal effects. A finite element approach has been adopted, and results provide useful relationships between mantle temperature and thickness of the oceanic lithosphere.

Computational challenges in modeling explosive volcanic eruptions

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Explosive volcanic eruptions are characterized by the injection in the atmosphere of a mixture of hot gases, liquid droplets and solid particles (pyroclasts) resulting from the fragmentation of the ascending magma and erosion of the volcanic conduit. The processes leading to explosive conditions are controlled by the non-linear magma rheology and by the rapid decompression of magmatic and hydrothermal volatiles during magma ascent. Driven by gas expansion throughout the conduit exit, the erupting mixture is injected in the atmosphere at high velocity, pressure and temperature, forming an under-expanded multiphase jet. The fate of the erupted, fragmented magma is then controlled by jet decompression dynamics, turbulent mixing and buoyancy reversal in the stratified atmosphere and by the mesoscale atmospheric dynamics.

A computational fluid dynamics approach to the modeling of explosive eruptions thus requires the ability to couple different domains and dynamics, and to deal with transient, polydisperse multiphase fluids, sub/supersonic flows, turbulence, thermal effects and complex 3D geometries and atmospheric wind fields. We discuss here some of the most recent advances in the physical and mathematical modeling of the pyroclastic dispersal process, and the perspectives for the large-scale numerical simulation of eruptive scenarios to the purpose of volcanic hazard assessment.

**MSP 21-23 - Mathematical methods in decisions, economics,
finance and games
I - II - III**

Our mini-symposium is devoted to the applications of Mathematics, Theoretical Physics and Theoretical Engineering in Decisions, Economics and Finance; with a particular emphasis to the applications of Games Theory. It is centered not only on the developments of the mathematical and theoretical methods of those fields but also upon the results which these methods can produce in Decisions, Economics and Finance and on their possible implementation by means of software realizations. Mathematical Economics, Political Economics, Economic Policy and Game Theory approached with the nonlinear functional analysis and Differential Geometry are also covered by our mini-symposium as well as the applications to the fundamental economic problems of allocating scarce resources among competing and cooperating agents, leading to considerations of the interrelated applications in Game Theory and the Theory of Optimization.

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Coopetitive models for a global sustainable green economy

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This paper provides coopetitive models for a global Green Economy, taking into account the environmental sustainability. In particular, we propose a series of differentiable coopetitive games - in the sense recently introduced by D. Carfi - to represent basic Green Economy interactions among a country c and the rest of the world w . Our games are linear and non-linear parametric perturbations of the classic Cournot duopoly. In the paper we offer the complete studies of the proposed models and in particular a deep examination of their possible coopetitive solutions: purely coopetitive; super-cooperative; TU purely coopetitive and TU super-cooperative.

Circulation of informational flows in organizations

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The formal structure of an organization is usually very different from the informal one. This occurs either because the leader of a group is rarely also the organization's manager, or because a person can be friends or not with his or her's co-workers and therefore, share information according to preferences. So what happens when information must be transmitted through the entire organization but the leader or manager doesn't agree with the information's contents, or when a worker doesn't like the co-worker he or she should communicate with? Can incomplete or erroneous information conveyed within an organization have negative influence on the organizational environment and the surrounding one? If so, how and to what extent? In order to have a sustainable development how should the information had been transmitted? In order to answer these questions, this research uses concept known from Decision Theory and Game Theory, because usually all organizations have a certain number of rules or beliefs, called organizational culture, that must be followed by all it's members. Thus, each and every single member, subgroup and group of an organization is expected to follow these beliefs and act accordingly, at least at formal level. We will start by studying one of the subgroups of a organization in order to find a behavior pattern. Then, following the concept of self-similarity we will use the behavior pattern of the subgroup and build a mathematical model that will lead us to an approximate behavior scenario of the entire organization when an information is transmitted. By studying this scenario we can estimate the information's flow effects upon the organizational environment on one hand and upon the surrounding environment itself on the other hand.

The coherence of anti-crisis solutions in Greece: effects and negative externalities

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Due to the fact that the World Economy is far from being recovered, or more realistically said, is far from reaching a recovery state, Europe has, in this moment, a first-row seat in this theatre hall. The problem of sovereign debts is still far to be resolved. One of the starting points in chain reaction was the Greek Scenario. In this paper we will use an interdisciplinary approach to study the anti-crisis policies applied in Greece since the beginning of the crisis in 2008, until the moment of speaking, and also, what remains to be done in order to avoid the spreading of this *cancer disease* through negative externalities into the *PIIGS countries* through a complex systems analysis. The model used to develop this paper is based on the one presented by Mansury, Diggory and Diesboeck in the article Evolutionary game theory in an agent-based brain tumor model: Exploring the *Genotype-Phenotype* link.

Optimal participation in illegitimate market activities: complete Pareto analysis of 2-dimensional cases

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In this paper, we consider the quantitative decision problem to allocate a certain amount of time upon two possible market activities, specifically, a legal one and an illegal one. This problem was considered in literature by Isaac Ehrlich (in his seminal paper *Participation in Illegitimate Activities: A Theoretical and Empirical Investigation*, published in *The Journal of Political Economy*, in 1973). The mathematical model we propose and use is essentially a formal mathematical translation of the ideas presented by Ehrlich. On the other hand, our approach will allow to apply efficiently and quantitatively the Ehrlich qualitative model. Specifically, in this original paper, we apply the Complete Pareto Analysis of a Differentiable Decision Problem, recently introduced in literature by David Carfi, to examine exhaustively the above Ehrlich-kind decision problem: given by a pair $P = (f, >)$, where the function $f : T \rightarrow \mathbb{R}^m$ is a vector payoff function defined upon a compact m -dimensional decision (time) constrain T and with values into the m -dimensional payoff space \mathbb{R}^m , for some natural number m (in our case m is 2). So, the principal aim of this paper is to show how the Carfi's Pareto Analysis can help to face, quantitatively, the decision problems of Ehrlich-type, in some practical cases; our approach is also justified by the circumstance that the computational aspects were totally not considered by Ehrlich. Our methodologies and approaches permit (in principle), by giving a total quantitative view of the possible payoff space of Ehrlich-decision problems (and consequently, giving a precise optimal solutions for the decision-maker), to perform quantitative econometric verifications, in order to test the payoff functions chosen in the various Ehrlich models. In particular, we apply our mathematical methodology to determine the topological boundary of the payoff space of a decision problem, in order to find optimal strategies in the participation in such legal and illegitimate market activities. The theoretical framework is clarified and applied by an example.

Speculative attacks: game theory and possible defenses

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In this paper we analyze a model of speculative attack on government bond market, by means of Game Theory and, specifically, applying to financial market the Complete Analysis of Differentiable Games (introduced in literature by David Carfi); in particular we propose a methodology to stabilize the price of government bonds of countries in the European periphery. We will focus our attention on two economic operators: an Investment Bank or a Hedge Fund (after called Speculator) and the European Central Bank (ECB). The crisis in the European bond market shows us how the Speculator, our first player in the Game, can influence markets and gain from the creation of arbitrage opportunities. At the same time we propose that the European Central Bank, our second player, can freely purchase government bonds in order to stabilize their price. In this work the normative authority introduces a Tobin tax on financial transactions that hit only the extra profits from speculation. At the end of the Game we show that increasing the interest rate on government bonds increases the possibility for Speculator to achieve earnings and decreases the opportunity of ECB of stabilizing the price of government bonds without losses.

Algorithms for payoff trajectories in C^1 coepetitive games

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In 2009, D. Carfi presented a new procedure to determine the payoff space of normal-form differentiable games; then, this new procedure has been applied in some papers to numerically determine the payoff space of normal-form C^1 parametric games, in two dimensions. In this work, the Carfi's method has been pointed out and assumed with the aim of realizing an algorithm for the computational representation of the payoff trajectory in the case of coepetitive C^1 games. The application of our algorithm to several examples concludes the paper. Our analysis allows us also to pass from the analysis of the fundamental characteristic of normal-form games to their coepetitive extension, as illustrated in several applicative papers by D. Carfi.

Public pension system sustainability

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The paper studies the sustainability of public pay-as-you-go PAYG pension systems. In particular it analyses Notional Defined Contribution NDC systems, which are financed on a PAYG basis, but where the pension is linked to the contributions paid during the working life, with a notional account for each participant. It presents a stochastic model for a defined contribution pension scheme with a funded component, focusing on the demographic risk new entrants. A set of risk indicators for the financial sustainability of the fund is constructed. The paper also gives numerical examples where these indices are applied.

Teaching aystem analysis to jurists - future specialists in legal informatics

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The presentation is concentrated on gap-filling in specialists' formation process in legal informatics (crossing between jurisprudence and informatics). The formation process of any specialist in any interdisciplinary field is always very complex and complicate, all the more, if this concerns the person that is studying all the time towards a jurist but wants to become the jurist, specialized in legal informatics, - so, become the half-informatician too. The question: which discipline of informatics has the most importance for academic preparation of jurist, as if he were prepared also as authentic IT-ist? The answer: it's guiding jurist to systemic reasoning, at least to level of system analyst; this can be achieved using the simplest example of legal studio as system, and the first two phases of its automatization: analysis and design. Material is elementary and nevertheless supplies future specialist with a strong and precise understanding of systemic point of view, letting him learn further easily - how to create, apply, analyse and control the mathematical models for professionally oriented systems in the field of jurisprudence, searching solutions for functional problems and such of informational, material, financial data management in the ambient of legal professional activity by means of mentioned systems.

The countries' technological level

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The fundamental requirements of sustainable development introduce a multidimensional approach to the analysis of the technological level of the countries, based on the balance of different needs. Indeed, the economic sustainability requires that manufactured capital, natural capital, human capital, and social capital must be all maintained over the long term, while the conservation of ecosystems and natural resources is essential for sustainable economic production and intergenerational equity. Moreover, the social equity is the basic element of development, and is interrelated with environmental sustainability. All these consideration are related to the technological development and its evaluation in relation to the processes used in the production activities. In this paper the anergy percentage is suggested as a suitable indicator of the level of the technological development, in relation to the optimized use of energy. This quantity, which is not a universal indicator in relation to the environmental impact, can be used for economic and socio-political evaluation. As a matter of fact, the anergy percentage is related to the exergy lost during a process, so it can give information on the optimization level obtained by a technology or it can be useful to compare different technologies among them.

MSP 25-27 - Mathematical modelling in biomedicine I - II - III

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 biomedical applications. These will range from the mechanics of growing tissues and oncology, to cardiology and neuropathology, from epidemiology to diagnostic. Also the mathematical tools used cover a wide range such as continuum mechanics, reaction-diffusion equations, delay differential equations, inverse problems, optimal control, statistics, measure theory, multiscale methods,

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Modelling the mechanical response of growing cellular aggregates

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We first study the mechanical behaviour of multicellular aggregates, subjected to a given deformation, using an elasto-visco-plastic model, in order to reproduce the bio-mechanical experiments performed in [1]. We then consider the case of cancer-spheroid growth inside healthy tissue.

Cell aggregates are treated as porous materials, composed of cells, with water filling void spaces. The cellular constituent is responsible for the elastic and the plastic behaviour (due to the rearrangement of adhesive bonds between cells), while the liquid constituent is responsible of the viscous-like response. The process of growth is modelled as the mass uptake of the solid-phase from the fluid-phase and it implies a continuum change of tissue geometry and internal structure.

In order to incorporate the capability of cells to reorganize and to grow, we use the notion of multiple natural configurations [3].

Our purposes are (i) to map the change of geometry of tumour aggregates and the surrounding tissue, (ii) to model the effect of stress on tumour growth and (iii) to discuss the influence of cell reorganization, as introduced in [2], on the overall process.

1. Forgacs, G.; Foty, R.A.; Shafirir, Y. and Steinberg, M.S. 1998 *Viscoelastic properties of living embryonic tissues: A quantitative study*. Biophys. J., 74, 2227-2234 .
2. Giverso, C. and Preziosi, L. 2011 *Modelling the compression and reorganization of cell aggregates*. Math. Med. Biol. , doi:10.1093/imammb/dqr008.
3. Humphrey, J. and Rajagopal, K. 2002 *A constrained mixture model and remodeling of soft tissues*. Math. Mod. Meth. Appl. Sci. 12, 407-430.

Time delay between RR and RT heart beat intervals assessed by trend extraction of exercise test data

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The RR and RT time intervals extracted from the electrocardiogram measure respectively the duration of cardiac cycle and repolarization. The series of these intervals recorded during the exercise test are characterized by two trends: a decreasing one during the stress phase and an increasing one during the recovery, separated by a global minimum. We model these series as a sum of a deterministic trend and random fluctuations, and estimate the trend using methods of curve extraction: running mean, polynomial fit, multi scale wavelet decomposition. We estimate the minimum location from the trend. Data analysis performed on a group of 20 healthy subjects provides evidence that the minimum of the RR series precedes the minimum of the RT series, with a time delay of about 19 seconds.

Closed-loop control of plasma glycemia: a DDE model-based approach

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Exogenous insulin administration is the basic way to face the widespread disease of Diabetes Mellitus. To this aim, closed-loop approaches, though theoretically realizable according to the control theory results and to the recent technology concerning continuous glucose measurements and affordable insulin infusion pumps, require a careful and thorough testing ground on a virtual environment before arranging an in-vivo clinical setting of experiments. In this talk, a model-based control law for the plasma glycemia is evaluated by closing the loop on a virtual patient, whose model equations are different from the ones used to synthesize the control law. That means: a minimal model of the glucose-insulin system to design the insulin therapy, and a different, more detailed, comprehensive model to test in silico the control scheme. Uncertainties on the blood glucose measurements, as well as malfunctioning on the insulin delivery devices are considered, according to the standard technology, in order to obtain an effective benchmark for the closed-loop control and to show in fact the robustness of the proposed approach.

Simulating human cardiac electrophysiology with unstructured all-hexahedral spectral elements

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We discuss the application of the spectral element method to both the monodomain and bidomain equations describing propagation of cardiac action potential. Some key elements related to the accuracy and computation efficiency of the proposed approach are analyzed on some selected benchmarks and on a realistic whole heart model.

Numerical modelling of electromagnetic sources by integral formulation

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Analysis of electromagnetic (EM) transients can be carried out by employing a field approach in frequency domain, based on an appropriate integral equation. This approach is a powerful method for the analysis of EM antennas and scatterers. Recent work by the authors in modeling electromagnetic scattering in frequency domain are summarized. Thin-wire electric field integral equation has been handled and possible application in obtaining sources localization information are discussed. Moments method (MoM) is used and time domain analysis is also carried out by discrete Fourier transform. Different approaches have been considered by using direct MoM formulation. Simulation results obtained both via Galerkin and point matching procedures are discussed.

A Bayesian approach to magnetoencephalography in the frequency domain

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The inverse problem of Magnetoencephalography is to reconstruct neuronal currents from measurements of the brain magnetic field. A recent approach to this ill-posed problem is based on Bayesian inference techniques in the time domain, whereby the unknown currents can be reconstructed with a time resolution of around 1 ms. In some applications, the spontaneous oscillatory activity of the brain is of interest: depending on the frequency band and the brain areas involved, such activity can be classified according to a set of different so-called ‘rhythms’. In order to detect a specific rhythm, it suffices to determine its leading frequency, its location in the brain and its strength. Hence, in this talk, we propose a Bayesian approach in the frequency domain, as it appears more direct and effective for this kind of applications, as well as less expensive from the computational viewpoint.

FitzHugh-Nagumo equations with generalized diffusion to model biological neural networks

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The work we present belongs to the field of biological neural networks. Two are the important aspects that we take into account to describe the dynamics of signals within a neural network. Firstly, a biophysically meaningful dynamics of each neuron of the network has to be described. Secondly, the structure of connections among neurons have to be defined. To tackle these two issues we propose to consider the spatially-distributed FitzHugh-Nagumo model, as presented in [1], with a modified discrete version of the diffusion operator. Specifically, in the context of the graph theory, the new diffusion operator is constituted by the Laplacian matrix which provides a structure within the neural network making explicit the connections allowed among neurons. The issue of weighted connections is also taken into account. More precisely, maintaining the property of Laplacian matrices, a hierarchy of connections is built making the information process more or less strong at the local level. Several integrations of the presented model are done. Using the Strang splitting method, the non-linear terms of the equations are advanced in time by the Runge-Kutta method (ode45 solver in Matlab) whereas the diffusion term is advanced by the Crank-Nicolson method. In order to present different dynamics, several simulations are done and presented in movie format.

1. Scott, A.C. 1975 *The electrophysics of a nerve fiber*. Reviews of Modern Physics. 47(2), 487–533.

Optimal control of culling in epidemic models for wildlife

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Optimal control theory is applied to a system of ODEs modeling infectious diseases in wildlife. Culling (the removal of individuals from an infected population) is introduced as a strategy to eradicate the infection, and plays the role of control variable. The optimization criterion is to minimize both the number of infected animals and the cost of culling effort. Different forms of the objective cost function are considered, including quadratic control and linear control, and in the latter case the possibility of singular control is investigated. The optimality systems are solved numerically [1] and results illustrate which is the optimal strategy in different scenarios, depending on the virulence of the disease.

1. Lenhart, S. and Workman, J.T. 2007 *Optimal control applied to biological models*. Chapman & Hall /CRC Mathematical and Computational Biology Series.

A new probabilistic approach to crowd dynamics for applications in built environment

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Performances of real world pedestrian facilities, such as pedestrian loads on footbridges or walkway serviceability, are evaluated in probabilistic terms in the current engineering and architectural practice. Bearing this in mind, a new probability-based approach to the modeling of crowd flows is proposed. The position of each pedestrian in a given walking area is expressed in terms of a time-evolving probability measure, whose evolution law is deduced consistently with non-local anisotropic microscopic models of the behavior of single walkers, including mutual pedestrian interactions. This approach allows one to account for uncertainties in initial/boundary conditions of crowd flow, as well as to provide occupancy statistics, without making use of several repeated simulations based on random sampling algorithms.

A mathematical model for p53 nuclear accumulation

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The p53 protein plays an essential role in the physiological maintenance of healthy tissue integrity in multicellular organisms (regulation of cell cycle arrest, reparation pathways and apoptosis).

We developed a spatial PDE model of p53 intracellular dynamics in order to understand whether the introduction of space in p53 dynamics allows modelling emerging phenomena and to make precise the role of each protein in the two relevant compartments, nucleus and cytoplasm, in p53 dynamics.

We will introduce our model, a reaction diffusion system where we add the crossing of the nuclear membrane through a Kedem-Katchalsky boundary condition. We will present its main aspects and results (oscillatory behaviour, bifurcations, robustness) and some numerical results in the 2D case.

Non-icosahedral pathways for the expansion of icosahedral viral capsids: a coarse grained model

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In this talk we present a theoretical model for structural transitions of icosahedral viral capsids, and we suggest possible pathways for the expansion of the capsid. We describe the capsid as an assembly of rigid hexamers and pentamers. We take into account a repulsive interaction energy between the RNA and the capsid, that tends to expand the capsid, and a cohesive energy between the capsomers. A change of the chemical environment triggers the conformational change of the capsid and the competition between the cohesive and repulsive energy results in a transition front moving along the particle. This work suggests that capsid expansion in icosahedral viruses is unlikely to occur through an icosahedrally symmetric expansion, but rather through a low-symmetry cascade of events.

**MSP 28-31 - Mathematical problems in semiconductors and
related topics
I - II - III**

The minisymposium intends to offer an occasion to bring together researchers working in the field of transport of charge in semiconductors. Both modeling and simulation aspects are considered and a special interest is dedicated to applications and problems arising from the microelectronic industry. The main topics concern: classical and quantum kinetic and macroscopic models, thermal effects, numerical methods, coupling between devices and circuits, optimization in nanoelectronics, solar cells, organic semiconductors.

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Quasibound states and transport resonances in coherent transmission spectra of electron waveguides

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The mechanism of charge transport through a non-homogeneous electron waveguide is deeply affected by the coupling between quasibound and traveling states, both in the single-particle and in the few-interacting-particle regimes. We will review the general framework of the above mechanism and specifically address numerical simulations of three systems of relevant practical interest, namely the scattering amplitudes of a single quantum dot[1], the entanglement creation of a double quantum dot[2], and the transmission spectra of twisted electron waveguides[3]. When few interacting carriers are bound in the structure, the exact calculation of the transmission amplitude must include both electronic repulsion and correlation, and becomes a challenging task, due to the needs of considering the few-particle wave function for an open system: a generalization of the "quantum transmitting boundary method" (QTBM) to the multi-particle case has been developed and applied. On the other hand, quasibound states may strongly bias also single-particle spectra of quantum wires if their nonuniform transverse section couples the dynamics of quantum particles in different directions, as for a twisted wire: from the comparison of results obtained with the "complex scaling method" and the QTBM we single out the effects of the twist.

1. Bertoni, A. and Goldoni, G. 2007 *Phase lapses in scattering through multielectron quantum dots: Mean-field and few-particle regimes*. Phys. Rev. B 75, 235318.
2. Buscemi, F. Bordone, P. and Bertoni, A. 2011 *On demand entanglement in double quantum dots via coherent carrier scattering*. New J. Phys. 13, 013023.
3. Cuoghi, G. Bertoni, A. and Sacchetti, A. 2011 *Effect of quasibound states on coherent electron transport in twisted nanowires*. Phys. Rev. B 83, 245439.

Is the Wigner transport equation to be modified for open systems?

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A problem was recently arisen [1] on the applicability of the Wigner-function formalism to open systems. Specifically, it was shown that the artificial spatial separation between the device active region and the external reservoirs is intrinsically incompatible with the non-local character of quantum mechanics. This problem will be re-examined and critically discussed. In order to have current through a device we must assume a source injecting/collecting carriers at the boundaries. If this is modelled by a plane wave crossing the in-boundary, the electron coherence extends to infinity. It will be shown that in such a case the Wigner transport equation, as usually written, does not hold. The example of a scattering state hitting a δ -like potential barrier will be thoroughly analysed.

1. Taj, D., Genovese, L. and Rossi, F. 2006 *Quantum-transport simulations with the Wigner-function formalism: Failure of conventional boundary-condition schemes*. Europhys. Lett. 74, 1060–1066.

Multiband transport in composite materials: effective mass theorem

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The effective mass approximation is a common assumption in solid state physics. It states that the motion of electrons in a periodic array of ions where some external non-periodic fields are also present, can be replaced by the motion of a fictitious particle with a modified mass in the presence of an effective smooth potential. The validity of this approximation relies on the observation that the period of the crystal lattice is usually small with respect the characteristic length of the non-periodic electrical or magnetic fields. In this contribution, we assume that that the electrons are confined in a lattice where the ionic potential is not strictly periodic. This situation models the more realistic case of a non-uniform semiconductor whose chemical-physical composition varies at the macroscopic scale. We perform a rigorous mathematical limit where the distance between the atoms of the lattice goes to zero (homogeneization limit). In the presence of composite materials, this limit justifies the use of an effective mass approximation with non-uniform effective mass. The study is performed within the kp multiband envelope function framework.

Two spinorial drift-diffusion models for quantum electron transport in graphene

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We will briefly describe two drift-diffusion models for quantum transport of electrons in graphene. The derivation is based upon the Minimum Entropy Principle (see [1] for details): considering the Wigner equations as the kinetic model for the system, we take moments of them and we close the resulting fluid-dynamic equations by choosing the Wigner distribution as a minimizer of a suitable quantum entropy functional. In order to obtain explicit models we make two assumptions: the usual semiclassical approximation and an ad-hoc hypothesis, the Low Scaled Fermi Speed (LSFS) approximation. We will briefly show some analytical results concerning one of the two models: existence of solutions, entropicity, uniform bounds on the moments, asymptotic behaviour and (under further assumptions) uniqueness of the solutions. Finally we will quickly present some numerical results related to both models.

1. Degond, P. and Ringhofer, C. 2003 *Quantum moment hydrodynamics and the entropy principle*. Journal of Statistical Physics 112, 587628.

On the two-temperature energy-transport model for semiconductors

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We consider an energy-transport model for semiconductors for the following unknowns: the electron number density n , the electron temperature T , the lattice temperature θ , and the electric potential ϕ . In the steady-state one-dimensional case, after scaling, the system can be written as follows:

$$J_x = 0, \tag{1}$$

$$J = n\phi_x - (nT)_x, \tag{2}$$

$$\left(\frac{5}{2}TJ - \kappa T_x\right)_x = J\phi_x - \frac{3}{2\tau}n(T - \theta), \tag{3}$$

$$(-\kappa_L\theta_x)_x = \frac{3}{2\tau}n(T - \theta) - \frac{1}{\tau_L}(\theta - 1), \tag{4}$$

$$\phi_{xx} = n - D, \tag{5}$$

with $x \in (0, 1)$. Here, J is the current density, κ and κ_L the electron and phonon thermal conductivities, respectively, τ and τ_L the electron and phonon energy relaxation times, $D(x)$ the doping profile. We assume the following physics-based boundary conditions:

$$n(0) = n_l, \quad n(1) = n_r, \tag{6}$$

$$T(0) = \theta(0), \quad T(1) = \theta(1), \tag{7}$$

$$\kappa_L\theta_x(0) = \frac{1}{R}(\theta(0) - 1), \quad -\kappa_L\theta_x(1) = \frac{1}{R}(\theta(1) - 1), \tag{8}$$

$$\phi(0) = 0, \quad \phi(1) = \phi_r. \tag{9}$$

For the above problem we establish a first existence and uniqueness result, under the assumption of smallness of the relaxation times τ , τ_L , and of the parameter $\delta := |n_r - n_l| + |\phi_r|$, related to the boundary conditions.

Simulation of 2D nanoscale double-gate MOSFETs including crystal heating

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A nanoscale double-gate MOSFET is simulated by using a model based on the maximum entropy principle (MEP) [1], [2] by including also the heating of the crystal lattice [3], [4]. The influence of this latter on the electrical performance of the device is addressed.

1. Camiola, V. D. and Mascali, G. and Romano, V. 2012 *Numerical simulation of a double-gate MOSFET with a subband model for semiconductors based on the maximum entropy principle*, Continuum Mech. Thermodyn. (at the present time available as published online).
2. Mascali, G. and Romano, V. 2012 *A non parabolic hydrodynamical subband model for semiconductors based on the maximum entropy principle*, Mathematical and Computer Modelling 55, 1003–1020.
3. Romano, V. and Zwierz, M. 2010 *Electron-phonon hydrodynamical model for semiconductors*. ZAMP 61, 1111–1131.
4. Romano, V. and Rusakov, A. 2010 *2d numerical simulations of an electron-phonon hydrodynamical model based on the maximum entropy principle*. Comput. Methods Appl. Mech. Engrg. 199, 2741–2751.

Hydrodynamical models for compound semiconductors

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In semiconductors, the charges mainly contributing to current are the electrons which occupy states around the minima of the lowest conduction bands and the holes around the maxima of the highest valence bands [1]. Therefore it is fundamental to build models which make use of the best possible approximation of the energy dispersion relations of these charges. Here we present a hydrodynamical model using of a generic expression for the dispersion relation, which comprehends as particular cases the Kane ellipsoidal approximation [2] and the warped approximation. The model is obtained starting from the Boltzmann transport equations for each charge population, taking the moments of these equations and closing the resulting macroscopic equations by means of the maximum entropy principle.

1. Jacoboni, C. 2010 *Theory of Electron Transport in Semiconductors*. Springer.
2. Ali, G., Mascali, G., Romano, V., Torcasio, R. C. 2012 *A hydrodynamic model for covalent semiconductors with applications to GaN and SiC*. Acta Applicandae Mathematicae, accepted for publication.

Hydrodynamic simulation of silicon nanowires

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Silicon nanowire (SiNW) devices have attracted significant interest due to their potential to function as logic devices [2], thermoelectric devices [1, 3], sensors [5]. As the silicon body diameter shrinks, the electronic states become subject to quantization because of the two-dimensional quantum confinement. The investigation of these devices by means of numerical simulations can be very informative.

Recently, a hydrodynamic model for silicon quantum wires has been developed by taking the moments of the multisubband Boltzmann equation, coupled to the Schrödinger-Poisson system [4]. Explicit closure relations for the fluxes and production terms have been obtained by means of the Maximum Entropy Principle of Extended Thermodynamics, including scattering of electrons with acoustic and non-polar optical phonons.

The obtained system of partial differential equations (PDEs), which we have verified to be of hyperbolic type, is solved by using a Runge-Kutta scheme, which is widely used for the time integration of PDEs of diffusion-convection type. This scheme, combined with WENO spatial reconstructions, avoid the onset of spurious numerical oscillations arising near discontinuities of the solution.

Applications to a $n^+ - n - n^+$ silicon diode are presented.

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2. Cui, Y., Lieber, C., 2001, *Functional nanoscale electronic devices assembled using silicon nanowire building blocks*. Science 291, 851853 .
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Scalable numerical algorithms for transient simulation of power electronics devices

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The numerical simulation of large area semiconductor devices for power electronics applications, such as Phase Control Thyristors (PCTs) or Bimode Insulated Gate Transistor (BIGTs) requires full-scale 3D simulations. Commercial 3D TCAD simulators, are mainly focused on the numerical modeling of CMOS devices and therefore most of the effort of their developers is aimed at correctly capturing the complex physical phenomena that affect charge transport at the nanoscale, rather than on providing the computational efficiency required for the simulation of large devices with complex geometries. For this reason MOX and ABB initiated a collaboration aimed at studying algorithms for large scale simulation of power electronics devices focusing in particular on their scalability for deployment on high performance parallel computing architectures. With this aim we developed an experimental TCAD simulator based on the in-house finite element library LDGH already in use at MOX and we tested its scalability with particular emphasis on the performance of iterative solution strategies for nonlinear equations.

Thermoelectric effects in silicon quantum wires

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A hydrodynamic model for silicon quantum wires is formulated by taking the moments of the multisubband Boltzmann equation [1], coupled to the Schrödinger-Poisson system. Explicit closure relations for the fluxes and production terms (i.e. the moments on the collisional operator) are obtained by means of the Maximum Entropy Principle of Extended Thermodynamics [2], including scattering of electrons with acoustic and non-polar optical phonons. By using this model, thermoelectric effects are investigated [3].

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Electron transport in one-walled carbon nanotube FET's

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We present an effective mass model, derived in [1], describing the ballistic transport of electrons in ultra-scaled confined nanostructures. Due to the strong confinement, the crystal lattice is considered periodic only in the one dimensional transport direction and an atomistic description of the entire cross-section is given. The model consists of a sequence of 1D device dependent Schrödinger equations, one for each energy band, which retain the effects of the confinement and of the transversal crystal structure. In order to model Field Effect Transistors, self-consistent computations include the resolution, in the whole 3D domain, of a Poisson equation. Simulations of the electron transport in semiconducting one-walled carbon nanotubes are presented, using a classical-quantum hybrid strategy. The ballistic effective mass model is used only in the active region, and it is coupled to a drift-diffusion model (obtained for strongly confined nanostructures in [2]) in the source and drain regions.

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Multiscale modeling and simulation of organic solar cells

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In this lecture, we propose and investigate a two-scale model of heterojunction organic solar cells (OSCs) [1]. The microscale model is a PDE/ODE system describing bulk excitation/transport phenomena and interfacial dissociation/recombination processes. The macroscale model is obtained by averaging the mass balance equations in the normal direction across the interface thickness, giving rise to nonlinear transmission conditions parametrized by the interfacial width and depending locally on the electric field magnitude and orientation. Macroscale simulations of 2D OSCs with complex interface morphologies show that the device performance is determined not only by the total interface length but also by its shape.

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Numerical method for a nanoscale DG-MOSFET

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By now for mathematical description of physical phenomena taking place in semiconductor devices one can apply the so-called hydrodynamical MEP (Maximum Entropy Principle) model. This model is a quasilinear nonstationary system of conservation laws obtained from the moment system of the Boltzmann kinetic equation (see [1], [9]). In this work we consider MEP model describing the charge transport process in DG-MOSFET transistor (see [8]).

In our previous works we have proposed a new technology for constructing the numerical algorithms for MEP model (see [3], [4], [5], [6], [7]). This technology uses the ideas of unsaturated schemes and method of lines (see [2]), the stabilization method, the interpolation polynomial with nodes in zeroes of Chebyshev's polynomial, the spline-function technique and the sweep method. It allows us to overcome the computational complexities caused by the presence of small parameters in MEP model and by the nonlinearity of its equations.

Now we apply this technology for solving the problem of charge transport in DG-MOSFET. This problem requires an essential expansion of the proposed ideas because of the structure of the transistor. After all modifications we construct a new effective algorithm, implement it and obtain the numerical solution of the considered problem.

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Recent advances in the spherical harmonics expansion of the Boltzmann transport equation

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Since typically employed macroscopic transport models are invalid in the deca-nanometer regime, accurate semiclassical simulation of carrier transport in semiconductors requires the solution of Boltzmann's transport equation. To overcome the deficiencies of stochastic Monte Carlo techniques, a deterministic solution approach based on a spherical harmonics expansion (SHE) has become increasingly attractive over the last years [1]. Unfortunately, the high computational effort of the SHE method has so far prevented its application to 3D geometries. We refine the SHE method by suggesting and evaluating adaptive variable-order expansions, a system matrix compression scheme for keeping the memory consumption at high expansion orders moderate, a parallel preconditioner for accelerating the solution of the resulting system of linear equations, and demonstrate an efficient implementation of the proposed algorithms on unstructured grids. The combination of these techniques allows for the efficient solution of higher-order expansions not only in low-dimensional devices, but also in the uncharted 3D regime.

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Semiconductor spintronics in a participating phonon medium: macroscopic equations

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A new model, based on an asymptotic procedure for solving the spinor kinetic equations of electrons and phonons is proposed, which gives naturally the displaced Maxwellian at the leading order. The balance equations for the electron number, total energy density, total momentum for the whole system constitute now, together with Poisson's equation, a system of four equations for the electron chemical potential, the temperature of the system, the drift velocity, and the electrical potential. In the drift-diffusion approximation the constitutive laws are derived and the Onsager relations recovered. Moreover an equation for the evolution of the spin density is added, which account for a general dispersion relation. The treatment of the spin-flip processes, derived from first principles is new and leads to an explicit expression of the relaxation time as a function of the temperature.

Hydrodynamic model for 2D-3D electron gas

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The main aim of the paper is to develop a hydrodynamical model for carrier transport in a nanoscale silicon MOSFET.

In a MOSFET the gate voltage and the energy barrier at the Si/SiO interface confine carriers near the oxide-silicon interface and a two dimensional electron gas (2-DEG) is formed. We consider the case where a 3-DEG coexists with the confined 2-DEG, formulating an energy transport model by using the maximum entropy principle.

MSP 32 - Networks and optimization

The recent surge in the network modeling of complex systems has set the grounds for new advances on the study of fundamental and applied aspects of optimization in collective behavior. Network models are applicable to an enormous variety of problems such as decision problems in the industrial sector, where optimization problems need to be solved efficiently and effectively. Some of these decision problems are really physical problems, for example, involving logistics, transportation or commodity flows. The family of network optimization problems includes the following prototype models: assignment, critical path, max flow, shortest path, transportation, and min cost flow problems. These problems are typically modeled through a series of network of arcs and nodes.

This Minisimposium presents an overview of results in this field and includes articles from various domains in which optimization manifests itself, including physical, biological, social, and technological networked systems. According to the nature of the talks, theoretical and computational issues are discussed.

The minisimposium is organized as follows, four topics are proposed:

1. Topological modeling of malware propagation in networks by an algorithm to reveal the more vulnerable nodes.
2. Existence results for non convex variational problems in L^∞ , necessary and sufficient conditions for the existence of solutions to the non level convex variational problems.
3. A mathematical model for container assignment optimization on an intermodal networks (maritime/inland component) able to minimize the sum of the total travel times for containers traveling on the networks.
4. A model that represents a neural network of Hippocampal CA1 brain region by using a parallel computing methodologies for simulations.

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Topological modeling of malware propagation in networks

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The spreading of dangerous malware (mal-icious soft-ware) [1] [2] in networks of electronics devices has raised deep concern, because from the ICT networks infections may propagate to other Critical Infrastructures producing the well-known domino effect. There are basically two diffusion strategies: the targeted intrusion and the cooperative search. As a side effect of the cooperative search, the malware will spread in the network like a disease (the "epidemic" spreading); the propagation of the infection follows the epidemic spreading model. Many actually research has suggested that the maximum eigenvalue of the adjacency matrix of the network could act as a threshold for the malware's spreading [3]. In this paper we study the Italian Internet Autonomous System simulating the diffusion of a worm, verifying the theoretical threshold; then we show how to choose in a suboptimal way the set of most influential nodes to protect with respect to the spectral paradigm. We present our bio-inspired algorithm, that is fast and outperforms topological measures as degree, closeness, betweenness, k-core, and we have applied it to a real network infected by StuxNet [4], textit[5]. During the numerical simulation on this real ICT network AV11 was able to stop the spreading of StuxNet.

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2. Wang Y., Chakrabarti D., Wang C. , Faloutsos C., 2003 Epidemic spreading in real networks. *SRDS Conference*.
3. Weaver N., et al., 2003 A Taxonomy of Computer Worms, *WORM03, October, Washington, DC, USA*.
4. Falliere D., 2010 Symantec report on StuxNet see: *www.symantec.com*
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A mathematical model for container assignment optimization on intermodal networks

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In this talk we propose a mathematical model for container assignment optimization on an intermodal network able to minimize the sum of the total travel times for containers traveling on the network. In this model we address both the maritime and the inland component, taking into account port characteristics as accessibility, loading/unloading and duty check times. The innovation of the proposed approach is twofold. First of all, we address the container assignment problem in its wholeness, through a realistic representation, instead of considering simplified versions of the problems, representing only parts of the distribution process. Second, we introduce a frequency based assignment criteria, which allow the model to identify more attractive paths connecting each origin-destination pair, and to proportionally split the flow among them in order to find an equilibrium between actual travel times (sailing times) and ports congestion. The proposed model may become a powerful tool, for shipping companies, to identify the most convenient routes for their expedition and, for ports authority, to analyze how the reduction of loading/unloading and duty check times may increase their port competitiveness.

Existence results for non ‘convex’ variational problems in L^∞

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Necessary and sufficient conditions for the existence of solutions to the ‘non level convex’ variational problems

$$\inf \left\{ \sup_{x \in \Omega} f(\nabla u(x)) : u \in u_0 + W_0^{1,\infty}(\Omega) \right\}$$

are provided. This result extends to the scalar supremal setting the theory started by [1] in the integral setting (see [2], [3] for a detailed analysis in the integral vectorial case).

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A parallel biological neural network of hippocampus region on GPU

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In [1] is showed that Scientific and Parallel computing methodologies are effective approaches to speeding up simulations of neural networks. Recent works address the problem of how efficiently modifying and implementing computational neural models on graphic processor units (GPUs). In [2] a model of Izhikevich neural network on a single GPU is developed. In [3], is constructed a framework for the modelling of both Hodgkin-Huxley and Izhikevich models in a two-layer network, used for image recognition. The main difficulty in achieving computational models of biological neural networks is that, increasing the complexity of these, we have a growing computational burden. Hence, the practical question is how to move a working network model from a single processor to parallel hardware, in order to exploit the computational power of multiple processors, that run simultaneously, and large amounts of total memory. In this talk we propose algorithms and strategies for implementing a biological neural network of Hippocampus brain region on a NVIDIA FERMI GPU architecture. The main goal will be the re-engineering of the computational models introducing the CUDA GPU programming methodology.

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**MSP 33-37 - New problems arising in mathematical modeling
of smart and biological materials
I - II - III - IV - V**

The Minisymposium is devoted to most recent results concerning mathematical models, with particular interest in smart and biological materials.

Notably, challenging analytical problems are originated from applications; indeed, *new* materials are more and more widely studied since they are used in a variety of different environments. Specifically, in recent years there has been a growing interest, on one hand, in materials with memory, and smart material in general, and, on the other hand, in biological materials. Indeed, all these materials exhibit crucial physical properties; in the case of materials with memory their behaviour depends on time not only through the present time but also through their past history. This peculiarity leads to the use of such materials in various different applications, like in biomedical tools and, in general, in sensors and actuators. Also biological materials require new analytical instruments to be modeled. More generally, other problems originating from different areas of biology as well as of medicine are of interest. The Minisymposium aims to bring together researchers who are investigating mathematical problems arising in modeling of such materials.

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Boundary controllability and source reconstruction in a viscoelastic string under external traction

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Treatises on vibrations devote large space to study the dynamical behavior of an elastic system subject to known external tractions. In fact, usually a “system” is not an isolated body but it is part of a chain of mechanisms which disturb the “system” for example due to the periodic rotation of shafts. This kind of problem has been rarely studied in control theory. In the specific case we shall study, the case of a viscoelastic string, the effect of such external action is on the horizontal component of the traction, and so it affects the coefficients of the corresponding wave type equation, which will be time dependent. The usual methods used in controllability are not naturally adapted to this case. For example at first sight it might seem that moment methods can only be used in case of coefficients which are constant in time. Instead, we shall see that moment methods can be extended to study controllability of a viscoelastic string subject to external traction and in particular we shall study a controllability problem which is encountered in the solution of the inverse problem consisting in the identification of a distributed disturbance source.

Stabilization for nonlinear integro-differential equations with weakly singular kernels.

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In this talk we will show stabilization results for nonlinear abstract evolution equations in the presence of a convolution integral term.

For concrete problems, e.g. the motion of some viscoelastic materials, the effects of the past time cannot be neglected: in the partial integro-differential equations describing the motion, the integral term just represents the memory of the past.

We will give decay estimates for the solutions when the convolution kernels are allowed to be weakly singular functions (integrable functions, singular at "t=0") and satisfy sign conditions consistent with thermodynamical restrictions.

Our main tools are coercive estimates, properties of positive definite kernels and the multipliers method: we succeeded in finding multipliers which work even in the presence of integral terms.

Joint work with Piermarco Cannarsa.

Discrete observability

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In the framework of a classical theorem due to Ingham, we will discuss some aspects of observability problems when the observation is given at a finite number of points of the given time.

The talk is based on joint works with Vilmos Komornik.

Some existence and uniqueness results in viscoelasticity: connections with free energies

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Integro-differential model problems arise in viscoelasticity. Here, some existence, and, possibly uniqueness, results recently obtained in joint work with V. Valente and G. Vergara Caffarelli, in the case, in turn, of a magneto-viscoelasticity problem [3], [4], or of a singular viscoelasticity problem [5] are considered. The connection between analytic results and the choice of suitable free energies is pointed out. Furthermore, the problem of the choice of the free energy, studied in various different physical models, in joint work with G. Amendola and A. Manes [1,2], is also considered. In particular, free energies in viscoelastic solids and fluids, [2], are also mentioned emphasizing their analytical implications as far as asymptotic behaviour of solutions is concerned.

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A phase transitions model for shape memory polymers

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We introduce a new predictive model for shape memory effects occurring in polymers. In spite of the great importance such materials have in new technologies and applications, a very few mathematical literature have been developed. Shape memory polymers may be deformed at some temperature and then recover their original shape just by thermal actions. This is not so far from shape memory alloys. However, the process on the basis of this effect is fairly different (mainly it is based on some order structure of the polymers chains), so that a completely new model has been introduced. Starting from experimental data we have introduced energy and dissipation functionals to get constitutive relations fitting with experiments. hence, by a generalized version of the principle of virtual powers we have recover an evolution PDE system for which we investigate existence of solutions. This research is developed in a collaboration with the Research Center on polymers of Versalis, Basic Chemicals & Plastics Research Center (ENI).

Free energies and phase transitions in materials with hysteresis

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A lot of mathematical models for magnetic hysteresis can be found in the literature, many of which are exhaustive and fit for applications (see, for instance, [1] and [2]). Unfortunately, none of them is able to describe the temperature-induced phase transition between the paramagnetic and the ferromagnetic regime. Recently, some efforts have been made in order to apply the Ginzburg-Landau theory in this direction [3]. In the talk we present a new approach to paramagnetic-ferromagnetic transition which involves a suitable order parameter related to the remnant magnetization. Starting from the skeleton curve description and exploiting the minimum (Gibbs) free energy representation, we are able to highlight the role of the Ginzburg-Landau equation when phase transitions in materials with hysteresis are involved. In particular, applications to ferrofluids and magnetic shape-memory alloys are expected.

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On a modified viscous Cahn-Hilliard type system

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A system modelling phase segregation that is similar to the viscous Cahn-Hilliard system is studied from the mathematical point of view. The talk regards a number of results in several directions (well-posedness, long-time behavior, asymptotic analysis with respect to a small parameter, optimal control) that the author recently obtained in collaboration with P. Colli, J. Sprekels and P. Podio-Guidugli.

Modelling of active particles in a mixture of fluids

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The motion of a cell population within an extracellular fluid is modelled by viewing cells, fluid and chemical attractant (or chemical factor) as constituents of a mixture. The cells are regarded as active (or self-propelled) particles. Their geometric structure is represented by a vector \mathbf{p} directed along a privileged direction of the cells. The evolution of \mathbf{p} is affected by the stretching of the fluid and the gradient of the attractant. The pertinent equations are the continuity equations for all constituents and the equations of motion for the fluid and the attractant. Because of the active character, the velocity of the cells, relative to the fluid, is modelled by a function of \mathbf{p} and of the gradient of the attractant. Relations with some classical mathematical models of related biological systems [1-3] are investigated.

1. Bellomo, N., De Angelis, E. and Preziosi, L. 2003 *Multiscale modeling and mathematical problems related to tumor evolution and medical therapy*. J. Theor. Med. 5, 111–136.
2. Hill, N. A. and Pedley, T. J. 2005 *Bioconvection*. Fluid Dyn. Res. 37, 1–20.
3. Valdés-Parada, F. J., Porter, M. L., Narayanaswamy, K., Ford, R. M. and Wood B. D. 2009 *Upscaling microbial chemotaxis in porous media*. Adv. Water Resour. 32, 1413–1428.

Modeling magnetostriction with phase change

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I shall report on some variational modeling of magnetostrictive effects in solids [1], especially in shape memory crystals. The idea is that of flagging the different phases (that is the different crystallographic variants) via the corresponding easy axes of magnetization. Different modeling regimes will be addressed and the corresponding existence, approximability, and control analysis will be outlined [2,3].

This is joint work with F. Auricchio, A. Reali, A.-L. Bessoud, and C. Zanini.

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2. Bessoud, A.-L. and Stefanelli, U. 2011 *Magnetic Shape Memory Alloys: three-dimensional modeling and analysis*. Math. Models Meth. Appl. Sci. 21, 1043–1069.
3. Stefanelli, U. 2012 *Magnetic control of magnetic shape-memory crystals*. Phys. B 407, 1316–1321.

A Ginzburg-Landau model in superfluidity

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We propose a thermodynamically consistent model to study the superfluid-normal phase transition in liquid helium, accounting for variations of temperature and density. According to the Ginzburg-Landau theory, the (second order) phase transition is described by means of an order parameter, describing the concentration of the superfluid phase and emphasizing the analogies between superfluidity and superconductivity. We decompose the velocity of the fluid as the sum of a normal and a superfluid component and we assume that the normal component is compressible and the superfluid component satisfies an evolution equation similar to the differential equation governing the motion of the superconducting electrons inside a superconductor. With these assumptions, the usual phase diagram of liquid helium is recovered and the continuity equation leads to a dependence between density and temperature in agreement with the experimental data.

Asymptotic dynamics of nonlinear coupled suspension bridge equations

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The long-term dynamics of a doubly nonlinear abstract system is analyzed. In particular, for a special choice of the nonlinear terms, the system describes the motion of a suspension bridge where the road bed and the main cable are modeled as a nonlinear beam and a vibrating string, respectively, and their coupling is carried out by nonlinear springs. The set of stationary solutions turns out to be nonempty and bounded in the energy norm. As the external loads vanish, the null solution of the system is proved to be exponentially stable provided that the axial load does not exceed some critical value. Finally, the existence of a bounded global attractor of optimal regularity is proved in connection with quite general nonlinear terms, exploiting a particular decomposition of the associated semigroup and bootstrap arguments (see [1], [2]).

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2. Giorgi, C., Pata, V. and Vuk, E. 2008 *On the extensible viscoelastic beam*. Nonlinearity 21, 713–733.

Some qualitative results in the mixtures of thermoelastic solids

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In this talk we present a model governing the thermomechanical deformations for mixtures of thermoelastic solids. In particular we discuss the asymptotic behavior of the associated solutions under suitable assumptions on the constitutive constants related to the mixtures.

Reconstruction of a convolution kernel in a parabolic problem with a memory term in the boundary conditions

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We consider a parabolic problem of the form

$$\begin{cases} D_t u(t, x) = Au(t, x) + (h * Au)(t, x) + f(t, x), & (t, x) \in (0, T) \times \Omega, \\ Bu(t, x) + (h * Bu)(t, x) + q(t, x) = M(u)(t, x) - u(t, x), & (t, x) \in (0, T) \times \partial\Omega, \\ u(0, x) = u_0(x). \end{cases}$$

Here A is a linear strongly elliptic operator of the second order in the open subset Ω , B is a linear operator of the first order, h is a convolution kernel depending only on t , f , q and u_0 are known data. M is a nonlinear memory operator, that is, an operator that, at time t , depends only on the restriction of u to $(0, t) \times \Omega$. We suppose that h is unknown, together with u and want to reconstruct them. To this aim, we assume that, for every t the datum

$$\Phi(u(t)) = \int_{\Omega} \omega(x)u(t, x)dx$$

is given. In applications, a problem of this type is a model of an automatic control problem, based on a feedback device. We may also think of h as regulator that we have at disposal, in order to obtain the prescribed $\Phi(u(t))$.

An irreversible phase transition problem with a nonlinear heat flux law

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We deal with a phase transition problem characterized by an irreversible evolution and ruled by a nonlinear heat flux law. It is described by the following system

$$\partial_t \vartheta + \vartheta \partial_t \chi - \operatorname{div}(k(\vartheta) \nabla \vartheta) = (\partial_t \chi)^2 \quad \text{a.e. in } \Omega \times (0, T), \quad (1)$$

$$\partial_t \chi - \Delta \chi + \partial I_{[0, +\infty[}(\partial_t \chi) + \chi^3 - \chi \ni \vartheta - \vartheta_c \quad \text{a.e. in } \Omega \times (0, T), \quad (2)$$

$$\partial_n \vartheta = \partial_n \chi = 0 \quad \text{a.e. in } \partial \Omega \times (0, T), \quad (3)$$

$$\vartheta(\cdot, 0) = \vartheta_0 \quad \chi(\cdot, 0) = \chi_0 \quad \text{a.e. in } \Omega, \quad (4)$$

where Ω is a smooth bounded domain in \mathbb{R}^3 with boundary $\partial \Omega$, $T > 0$ is a given final time, ϑ stands for the absolute temperature, ϑ_c for the critical transition temperature, and χ for a phase variable. Moreover $\partial I_{[0, +\infty[}(\cdot)$, denoting the subdifferential of the indicator function $I_{[0, +\infty[}(\cdot)$ ($= 0$ if the argument is nonnegative, $= +\infty$ otherwise), forces $\partial_t \chi$ to be nonnegative and it renders the irreversible character of the evolution. Finally, the positive function k , representing the heat conductivity of the process, satisfies suitable growth conditions and can model the case of high temperature phenomena.

The derivation of (1)-(4) comes from the theory proposed by M. FRÉMOND [2]. The main analytical difficulty connected with this problem is due to the presence of the quadratic terms in (1) which can prevent to deduce global-in-time existence (and uniqueness) results. Also exploiting the proper features of the heat flux law (k is assumed to be positive and to behave like ϑ^p , $p \geq 2$ for large values of ϑ), we can work in a functional setting which is regular enough to deal with the nonlinearities of the system. We obtain a global-in-time well-posedness result [1].

1. Bonfanti, G. and Luterotti, F. *A well-posedness result for irreversible phase transitions with a nonlinear heat flux law*. Discrete Contin. Dyn. Syst. Ser. S, in print.
2. Frémond, M. 2002 *Non-smooth Thermomechanics*. Springer-Verlag, Berlin.

These results have been obtained in collaboration with:

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A phase-field model for shape memory alloys at macroscopic scale: uni-axial deformation tests under different control conditions

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We propose a model for the thermomechanical behaviour of a shape memory alloy based on a phase-field approach to the underlying martensitic phase transition [1]. The model is applied at the macroscopic scale and it is essentially apt to capture the one-dimensional mechanical behaviour; in fact, the effect of the martensitic phase transition has been included in terms of a uni-axial deformation along a fixed direction. In addition to the usual momentum balance equation, a time-dependent Ginzburg-Landau equation is introduced to describe the evolution of the phase; a central constitutive relation couples the phase to the deformation. Finally, the heat equation accounts for the non isothermal effects due to the phase transformation in a thermodynamically consistent way. The model has been implemented within a finite-element framework and the mechanical response of the model under different conditions is investigated in a number of numerical tests; the results obtained are analysed and compared to the experimental evidences available in literature.

1. D. Grandi, M. Maraldi, L. Molari, *A macroscale phase-field model for shape memory alloys with non-isothermal effects: Influence of strain rate and environmental conditions on the mechanical response*, Acta Materialia 60 (2012) 179–191.

Diffusion and current-voltage curves in potassium channels

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We consider the outflux of ions through a ion channel in a cell membrane. It is well known that such channels exhibit, among other peculiar features, the capability of selecting ions of preferred chemical species, e.g., K^+ over Na^+ .

The existence of an external voltage difference across the cell membrane has important effects on the total current through the channel. We examine the possibility to predict the behavior of the current-voltage curves on the basis of a model similar to the one in [1].

There we introduced a random-walk model where the channel is lumped to a two state stochastic point system, and gating of the channel (i.e., switching between closed and open phases) is achieved by means of changes in affinity for the (preferred) ions, following an idea in [2]. Differently from other models we take into account also the influence of diffusion in the cell. A mild modification is needed to take into account the effect of the trans-membrane voltage difference.

We shall compare the current-voltage behavior predicted by our model with experimental results.

1. Andreucci, D., Bellaveglia, D., Cirillo, E.N.M. and Marconi, S. 2011 *Monte Carlo study of gating and selection in potassium channels*. Physical Review E 84, 021920.
2. VanDongen, A.M.J. 2004 *K channel gating by an affinity-switching selectivity filter*. PNAS 101, 3248-3252.

Two-phase mass transfer in drug delivery systems: an application to the drug-eluting stent

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Biodegradable polymeric coatings on cardiovascular stents are commonly used for local delivery of therapeutic drug to diseased coronary arteries after stenting procedures. The stent-based drug delivery is not completely understood and the elution mechanism may be influenced by different concurrent processes. One of them is the structure of the arterial wall that is recognized constituted by a sequence of adjacent layers. The multilayered wall accounts for a relatively detailed structure for the macromolecular transport inside the biological tissues and provides a better description when compared with a homogeneous monolayered model in diffusion processes. Another aspect is the porous coating structure where the drug, initially present in solid phase, passes into the liquid phase and, as such, is released in the tissue. We define a characteristic transfer time and we solve the transient drug dynamics problem in the adjoining wall layers faced with the coating. The endothelium, intima, internal elastic lamina and media are all treated as homogeneous porous media and the drug release from the coating through them is modelled by a set of coupled partial differential equations. The local non-equilibrium mass transport in the coating is described by adding a solid phase equation containing a solid-fluid transfer term. A spectral decomposition method for a multi-layer configuration is used. Drug concentration level and mass profiles in each layer at various times are given and discussed. As long as built on a realistic set up, the current simulation is able to estimate the local concentration, offers an easy tool for computing useful indicators such as the residence time of a drug and can be used as a guideline for designing better delivery systems.

Nonlinear heat transport in nanosystems

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The aim of this presentation is to analyze some nonlinear effects arising in heat transport at the nanoscale, which are especially relevant because, due to the small size of the heat conductor, small temperature differences could lead to high values of temperature gradient.

Such effects are discussed on the basis of a weakly nonlocal and nonlinear heat transport equation and a dynamical nonequilibrium temperature [1,2].

Our study will concern not only the nonlinear effects arising by the dependence of the thermal conductivity, or of the specific heat, on the temperature, but also the ones due to terms in the heat transport equation which are nonlinear in the heat flux itself.

The consequences of nonlinearity are illustrated in different situations of practical interest, involving nanowires, carbon nanotubes, and graphene sheets. The thermodynamic aspects are considered as well.

1. V. A. Cimmelli, A. Sellitto and D. Jou, 2010 *Nonequilibrium temperatures, heat waves, and nonlinear heat transport equations*, Phys. Rev. B 81, 054301 (9 pages).
2. V. A. Cimmelli, A. Sellitto and D. Jou, 2010 *Nonlinear evolution and stability of the heat flow in nanosystems: Beyond linear phonon hydrodynamics*, Phys. Rev. B 82, 184302 (9 pages).

**MSP 38-39 - Nonlinear evolution equations: analytic and
geometric methods
I - II**

Integrable nonlinear evolution equations arise in many applications such as propagation of signals in optical fibers, water waves, Bose-Einstein condensation, two dimensional gravity, interface motions, propagation of deformations along the DNA chain. The Cauchy problem of such equations can be solved by the inverse scattering transform (IST), a nonlinear analogue of the Fourier transform, which translates the time evolution of the solution of the nonlinear equation into the more elementary time evolution of the scattering data. There exist continuous and discrete versions of such equations. Using a Marchenko integral equation or a Riemann-Hilbert problem to implement the final step of the IST, linear algebra methods can be used to derive explicit solutions. The IST can be derived from a Hamiltonian principle, leading to a geometrical approach to study the evolution of an integrable equation. The Hamiltonian structure of a physical model is, also in the nonintegrable case, a powerful tool for finding the symmetries of the system. In this context the integrability is encoded on a couple of different but compatible Poisson brackets for the same system which allows a geometric construction of the Hamiltonian function also.

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Coupled Maxwell-Bloch equations with inhomogeneous broadening for a 3-level system

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The phenomenon that describes the effect of a coherent medium response to an incident electric field, to which the medium is totally transparent and which undergoes lossless propagation, is known as self-induced transparency (SIT). SIT was first discovered by McCall and Hahn (1969) in the case of non-degenerate two-level atoms. Special solutions for the two-level system were found by Lamb (1971), while the initial value problem for the propagation of a pulse through a resonant two-level optical medium was solved by Inverse Scattering Transform (IST) in [1,2].

It is possible to formulate the SIT equations in the framework of the IST also in the case of a three-level system, as in [3]. While the associated scattering problem is the same as for the coupled nonlinear Schrödinger equation, the time evolution depends on asymptotic values of the material polarizability envelopes and is highly non-trivial.

This talk will address the solution of the initial value problem for the SIT equations for three level systems, for generic preparation of the medium, and describe its soliton interactions.

1. M.J. Ablowitz, D.J. Kaup, A. C. Newell, J. Math. Phys. **15**, 1852 (1974)
2. I.R. Gabitov, A.V. Mikhailov, V.E. Zakharov, Theor. Math. Phys. **63**, 328 (1985)
3. J.A. Byrne, I.R. Gabitov, G. Kovačič, Physica D **186**, 69 (2003)

Propagating two-dimensional magnetic droplets

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Recent results on propagating, solitary magnetic wave solutions of the Landau-Lifshitz equation with uniaxial, easy-axis anisotropy in thin (two-dimensional) magnetic films will be illustrated. These localized, nontopological wave structures, parametrized by their precessional frequency and propagation speed, extend the stationary, coherently precessing "magnon droplet" to the moving frame, a non-trivial generalization due to the lack of Galilean invariance. Propagating droplets move on a spin wave background with a nonlinear droplet dispersion relation that yields a limited range of allowable droplet speeds and frequencies. The droplet is found to propagate as a Nonlinear Schroedinger bright soliton in the weakly nonlinear regime. An iterative numerical technique is used to compute the propagating droplet's structure and properties. The results agree with previous asymptotic calculations in the weakly nonlinear regime. Furthermore, an analytical criterion for the droplet's orbital stability is confirmed. Time-dependent numerical simulations confirm the propagating droplet's stability when its frequency and speed lie within the allowable range.

1. M. Hofer and M. Sommacal, Propagating two-dimensional magnetic droplets, *Physica D* **241**, 890-901 (2012).
2. M. Hofer, M. Sommacal and T. Silva, Propagation and control of nano-scale, magnetic droplet solitons, *submitted to Phys. Rev. Lett.*
3. A. Kosevich, B. Ivanov and A. Kovalev, Magnetic solitons, *Phys. Rep.* **194**(3-4), 117-238 (1990).
4. B. Piette and W. Zakrzewski, Localized solutions in a two-dimensional Landau-Lifshitz model, *Physica D* **119**(3-4), 314-326 (1998).

Nonlinear propagation in optical fibers: a perturbation theory for the stochastic nonlinear Schrödinger equation

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One of the most relevant mathematical problems in fiber-optic communications is the statistical characterization of the received optical signal after propagation through the optical fiber. Indeed, the evaluation of the fundamental information-theoretic limits of the fiber-optic channel and the design of effective fiber-optic systems depend on the availability of an accurate and mathematically tractable statistical description of the optical signal and its evolution during propagation. In particular, when including dispersion, attenuation, Kerr nonlinearity, and in-line optical amplification, the propagation of the signal through the fiber-optic link is governed by the stochastic nonlinear Schrödinger equation.

This talk presents a general formulation of the problem, including some practical constraints on the equation parameters and the initial datum (the input signal) for relevant applications, and discuss a perturbation theory approach to its solution. In particular, starting from the exact analytical solutions obtained for specific propagation regimes, different perturbation methods—namely, regular, logarithmic, and combined regular-logarithmic—are proposed and compared to derive simple, yet accurate, approximated solutions of the general problem. Finally, some alternative approaches are briefly considered and discussed.

Integrable discrete nonlinear Schrödinger equations with vanishing and nonvanishing boundary conditions

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Discretizations of matrix nonlinear Schrödinger equations have the problem that the natural finite difference discretization of the matrix NLS equation leads to a nonlinear equation whose integrability is not obvious. This has led to the development of an inverse scattering transform scheme where the (focusing) discrete NLS solution $\mathbf{u}_n(t)$ is required to let $\mathbf{u}_n(t)\mathbf{u}_n(t)^\dagger$ and $\mathbf{u}_n(t)^\dagger\mathbf{u}_n(t)$ be nonzero multiples of the identity matrix, thus preventing a proper discretization of the Manakov system.

In this talk we explore various remedies. One is to discretize every single step in the IST, but in this case the nonlinear evolution problem might be difficult to formulate (although integrability is guaranteed). The other option is to apply central differencing (and not one-sided differencing as Ablowitz-Ladik did) in the matrix Zakharov-Shabat system, develop the direct and inverse scattering theory of the resulting system

$$iJ \frac{u_{n+1} - u_{n-1}}{2h} = [\lambda I_{N+M} + U_n]u_n,$$

stick in time factors, and apply the usual matrix triplet method to develop explicit discrete NLS solutions. We discuss some ideas of studying discrete nonlinear Schrödinger equations with solutions not vanishing as $n \rightarrow \pm\infty$.

Flutter and gradient catastrophe in vortex filament dynamics with axial flow

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Flutter type instability in the motion of a vortex filament in an incompressible unbounded Euler fluid is discussed. Within the localized induction approximation the origin of this phenomenon is in the gradient catastrophe for the dispersionless Da Rios system. This system describes the motion of a filament with slow varying curvature and torsion. Geometrically, the gradient catastrophe manifests as a rapid oscillation of a filament curve in a point that resembles the flutter of airfoils. In the point of catastrophe the curvature radius remains finite while the radius of osculating sphere blows up to infinity. Analytically, the catastrophe is the elliptic umbilic singularity in the terminology of the catastrophe theory. Its double scaling regularization is governed by the Painlevé-I equation. Deeper singularities, in particular the unimodular parabolical singularity X_9 , are also studied.

Gradient catastrophe and flutter type instability for the integrable extensions of the dispersionless Da Rios system arising in more general models of self-induced motion of filament which include axial velocity and other effects are considered too.

Solutions of vortex filament motion both in localized induction approximation and also with axial flow describe quasi conformal mappings on the plane.

1. Konopelchenko, B. and Ortenzi, G. 2011 *Gradient catastrophe and flutter of vortex filament dynamics*, J. Phys. A: Math. Theor. 44 432001
<http://iopscience.iop.org/1751-8121/labtalk-article/48066>

Numerical solution to the nonlinear Schrödinger equation

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The inverse scattering transform technique is used to develop a numerical procedure for solving the focusing nonlinear Schrödinger equation (NLS) $i q_t = q_{xx} + 2q|q|^2$, where $q(x, 0)$ is given. The procedure summarizes in: solving a Volterra integral equation to obtain the initial set of scattering data (which determines the initial Marchenko kernel); propagating the Marchenko kernel up to a time value \bar{t} ; eventually solve the set of integral Marchenko equations to obtain the solution to the NLS, i.e., $q(x, \bar{t})$ in a set of gridpoints $\{x_i\}$. Linear algebra and structured matrices techniques are used to speed up the procedure. We also propose a wide numerical experimentation and comparison with other numerical techniques.

An inertia ‘paradox’ for incompressible stratified Euler fluids

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The interplay between incompressibility and stratification can lead to non-conservation of horizontal momentum in the dynamics of a stably stratified, incompressible Euler fluid filling an infinite horizontal channel between rigid upper and lower plates. Lack of conservation occurs even though in this configuration only vertical external forces act on the system. This apparent paradox was seemingly first noticed by Benjamin (in 1986) in his classification of the invariants by symmetry groups with the Hamiltonian structure of the Euler equations in two dimensional settings, but it appears to have been largely ignored since. By working directly with the motion equations, the paradox is shown here to be a consequence of the rigid lid constraint coupling through incompressibility with the infinite inertia of the far ends of the channel, assumed to be at rest in hydrostatic equilibrium. Accordingly, when inertia is removed by eliminating the stratification, or, remarkably, by using the Boussinesq approximation of uniform density for the inertia terms, horizontal momentum conservation is recovered. This interplay between constraints, action-at-a-distance by incompressibility, and inertia is illustrated by layer averaged exact results and two-layer long-wave models.

Constructing multidimensional Fourier solutions of integrable and nonintegrable evolution equations

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I address nonlinear evolution equations (NEE) from the point of view of spatially periodic boundary conditions. The reason for this choice is dictated by applications in nonlinear wave physics, hydrodynamics and ocean waves. For integrable equations the solutions are in terms the inverse scattering transform and Riemann theta functions. Extending some of the soliton solution techniques to nonintegrable equations is the goal of this research. Can soliton theory be useful even for nonlinear evolution equations that are nonintegrable and which may also have chaotic solutions? At first blush this does not seem to be possible, but I show that even for nonintegrable equations some of the solitonic ideas are nevertheless quite useful. In particular I discuss how ordinary Fourier series and multidimensional Fourier series can be employed simultaneously to reduce a large class of NEEs to dynamical systems of the classical form

$$\dot{\mathbf{x}} = \tilde{\mathbf{A}}(\mathbf{x}, t)\mathbf{x}$$

I show how many of these systems have multiperiodic Fourier series solutions:

$$\mathbf{x}(t) = \sum_{\mathbf{n} \in \mathbb{Z}} \mathbf{x}_{\mathbf{n}}(t) e^{-i\mathbf{n} \cdot \boldsymbol{\omega} t + i\mathbf{n} \cdot \boldsymbol{\phi}}$$

Systems of this type may be classified as being near integrable and their dynamics can therefore be followed on a Riemann surface. For the class of NEEs which can be converted to an N -linear form the formulation is found to provide (1) tools for understanding the physics in terms of coherent structures such as solitons, rogue waves and vortices, (2) for the analysis of data from hydrodynamic systems and the ocean and (3) for the hyperfast numerical simulation of wave dynamics using multidimensional Fourier series. Many of the arguments in my talk have also been discussed in my book [1] and references therein.

1. Osborne, Alfred R. 2010 *Nonlinear Ocean Waves and the Inverse Scattering Transform*, Academic Press, Boston, 976 pages.

**MSP 40-41 - Numerical modelling for engineering applications
involving complex fluids and geometries
I - II**

Predicting the behavior of complex phenomena is a problem of paramount importance for both industrial and natural processes, in particular when dealing with complex fluids and/or complex geometries. This minisymposium aims at presenting paradigmatic applications where accurate mathematical models and sophisticated numerical methods have to be employed to guarantee reliable predictions. In particular, the following topics will be considered: chimera and mesh-less methods for CFD, dynamics of fluid membranes, numerical modelling of metal foams formation, flows in discrete fracture networks, underground and environmental fluid dynamical problems, numerical simulations of tissue engineering. The minisymposium aims at bringing together researchers in different fields of applied mathematics and will be the occasion both for a comparison of different state-of-the-art perspectives and techniques and a fruitful cross-fertilization of ideas.

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Algorithms for adaptive particle distributions and multi-resolution in SPH schemes

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The Smoothed Particle Hydrodynamics (SPH) is a lagrangian particle method. The meshless character of this numerical scheme makes it fundamentally different from conventional techniques and, in the context of violent free-surface flows, SPH permits to overcome some shortcomings of standard grid solvers. Notwithstanding that, algorithms to adapt automatically and locally the spatial resolution are still under development. Benefits and drawbacks of these algorithms are presented in this work. The first method discussed is the h-variable scheme [2]. Although this kind of scheme already exists, there is still a lot to do, mainly because stability is until now restricted to smoothly varying h, accuracy has to be closely controlled, and care is required to preserve exact local conservation of mass, momentum and energy. An alternative to the h-variable scheme is to consider a multi-block technique. The flow domain could be divided into blocks of various spatial resolutions. The main challenge is the transfer of information from one block to another across the interface. Finally, a particle packing algorithm is presented that initialises particle positions for generic geometries in such a way to achieve static equilibrium, eliminating the generation of spurious currents caused by the re-settling of fluid particles [1].

1. Colagrossi, A., Bouscasse, B., Antuono, M. and Marrone, S. 2012 *Particle packing algorithm for SPH schemes*, *Comp. Phys. Comm.*, In Press (Available online).
2. Nelson, R.P. and Papaloizou, J.C.B. 1994 *Variable smoothing lengths and energy conservation in SPH*, *Mon. Not. R. Astronom. Soc.* 270, 1–20.

URANSE Simulations of Complex Moving Bodies by means of Dynamic Overlapping Grids

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In applied hydrodynamics it is presently a general common task to simulate flow around complex shaped ships with moving appendages. As an example the simulation of a turning circle manoeuvre of a full-appended combatant ship is common in manoeuvrability studies. Nevertheless the accurate numerical simulation of turbulent, unsteady flow around a full appended maneuvering complex-shaped hull is a challenging task, because of the geometrical complexity of the appendages present and their relative movement, generating a very complex hydrodynamic flow.

Two (at least) are the key-features for a well resolved numerical simulation of this kind of problems: an accurate numerical method and a suited numerical grid.

The numerical model we adopt belongs to the numerical integration of the Unsteady Reynolds Averaged Navier-Stokes Equations (URANSE): it is based on a finite volume technique with pressure and velocity co-located at cell centers; for the viscous terms a standard second-order centered scheme is adopted, whereas for the inviscid part three different schemes can be chosen: a second-order ENO (essentially nonoscillatory) scheme, a third-order upwind scheme, and a fourth-order centered scheme; the physical time derivative in the governing equations is approximated by a second-order accurate, three-point backward finite difference formula. In order to obtain a divergence free velocity field at every physical-time step, a dual or pseudotime derivative is introduced in the discrete system of equations; the convergence ratio for the inner iteration is accelerated by means of local time stepping, an implicit Euler scheme with approximate factorization and a multigrid technique; many different turbulence models are available.

For a well resolved boundary layer turbulent flow a body-conformal grid is mandatory but for the complexity of the geometries studied (and their relative movements) it is not possible to use a simple structured multi-blocks grid: there is the necessity of more flexibility. To this aim we adopt a dynamic overset grid technique; each geometrical element of the whole geometry is discretized with a set structured body-conformal grid blocks with partial overlapping each others (Chimera approach).

In the full presentation details of our numerical approach will be explained. Some interesting applications will be presented highlighting pros and cons of our technique.

Metal foams formation: a numerical model

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Metal foams are special cases of cellular metals with closed cells. These materials attracts the attention of researchers and engineers, thanks to properties like damping, high capability of energy absorption, high stiffness and low weight, that make them suitable for a wide range of applications, in particular in the automotive industry. The high costs and the lack of control in the manufacturing process (in order to avoid foam-decay phenomena like drainage and coarsening) prevent the industrial production of this type of materials. During this talk, we will propose a phase-field model for the so-called powder metallurgical route for the foaming process. In particular, we will focus on the mathematical and numerical modeling of the expansion of the foam inside a mould. This will result in a Navier-Stokes-Cahn-Hilliard system of equations for a continuum medium (the foam) which occurs in two different phases: the liquid (the metal, which is incompressible) and the gas in the bubbles (the hydrogen, which is compressible).

Two and three dimensional simulation of flow and particle transport in porous media

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The simulation of fluid flow and particle transport in porous media finds important applications in many different fields, ranging from environmental and oil engineering to filtration and industrial chromatography. Different types of approaches exist and are generally classified by the length- and time-scales involved. Real industrial problems require the treatment of the porous medium as a continuum via the definition of porosity and permeability. However, these parameters are very difficult to be determined and therefore a strategy to identify them from pore-scale simulation is investigated here. Two and three dimensional geometries characterized by different degrees of complexity are created and studied using finite-element and finite-volume computational fluid dynamics codes. First the flow and particle transport around spherical grains arranged in a regular lattice is investigated. Then the analysis is extended to irregularly arranged spherical grains (of equal and different size) mimicking a realistic porous medium. Eventually geometries constituted by grains of realistic shapes are also considered. The accurate simulation of these systems require the solution of a number of mathematical and numerical challenges, related to computational geometry, mesh processing and discretization techniques. Particular attention is devoted to the assessment of two meshing strategies: highly irregular body-fitted meshes versus regular cartesian-based immersed-boundary approach.

Computational models for large contrast problems applied to microscale analysis of tissue engineered constructs.

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We aim to develop and validate suitable mathematical models and computational techniques for the interpretation and prediction of polymer scaffolded systems for engineered tissue growth, where a quantitative understanding of the interplay among geometry, flow perfusion, nutrient/waste mass transfer and cellular proliferation is required [1]. To succeed, we need to substantially simplify the interaction between image-based biomedical data and computational models based on PDEs. This will be achieved by means of the fictitious domain concept combined with the extended finite element method, leading to the approximation of contrast problems by means of a numerical scheme which does not require that the computational mesh conforms to the interface of discontinuity between coefficients [2,3]. A thorough stability and error analysis will be discussed for the case of diffusion-reaction equations. The robustness and the simplicity of implementation of the proposed scheme motivate its extension to time dependent problems with moving interfaces as well as to incompressible fluid dynamics. Perspectives and results along these directions will be also discussed.

1. R. Sacco, P. Causin, P. Zunino, M.T. Raimondi, A multiphysics/multiscale numerical simulation of scaffold-based cartilage regeneration under interstitial perfusion in a bioreactor, *Biomech. Model. Mechanobiol.*, Vol. 10 (2011), No. 4, pp. 577-589.
2. P. Zunino, L. Cattaneo, C.M. Colciago, An unfitted interface penalty method for the numerical approximation of contrast problems, *Appl. Num. Math.*, Vol. 61 (2011) No. 10, pp. 1059-1076.
3. E. Burman, P. Zunino, Numerical Approximation of Large Contrast Problems with the Unfitted Nitsche Method, *Frontiers in Numerical Analysis - Durham 2010, Lecture Notes in Computational Science and Engineering*, Vol. 85, 2012, Springer-Verlag, Heidelberg, Germany, ISBN 978-3-642-23913-7.

The role of membrane viscosity in the dynamics of fluid membranes

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Fluid membranes made out of lipid bilayers are the fundamental separation structure in eukaryotic cells. Many physiological processes rely on dramatic shape and topological changes (e.g. fusion, fission) of fluid membrane systems. Fluidity is key to the versatility and constant reorganization of lipid bilayers. Here, we study the role of the membrane intrinsic viscosity, arising from the friction of the lipid molecules as they rearrange to accommodate shape changes, in the dynamics of morphological changes of fluid vesicles. In particular, we analyze the competition between the membrane viscosity and the viscosity of the bulk fluid surrounding the vesicle as the dominant dissipative mechanism. We consider the relaxation dynamics of fluid vesicles put in an out-of-equilibrium state, but conclusions can be drawn regarding the kinetics or power consumption in regulated shape changes in the cell. On the basis of numerical calculations, we find that the dynamics arising from the membrane viscosity are qualitatively different from the dynamics arising from the bulk viscosity. When these two dissipation mechanisms are put in competition, we find that for small vesicles the membrane dissipation dominates, with a relaxation time that scales as the size of the vesicle to the power 2. For large vesicles, the bulk dissipation dominates, and the exponent in the relaxation time vs. size relation is 3.

An extended finite element optimization method for simulating discrete fracture network flows

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A new numerical approach for the computation of the 3D flow in a discrete fracture network [1], [2], [3], [4] not requiring the discretization of partial differential equations on complex 3D system of planar fractures will be described and analysed [5]. The discretization within each fracture is performed independently of the discretization of the other fractures and of their intersections. Independent meshing process within each fracture is a very important issue for practical large scale simulations making easier mesh generation and parallelization. Some numerical simulations are given to show the viability and efficiency of the method.

1. Cacas, M. C.; Ledoux, E.; de Marsily, G.; Tillie, B.; Barbreau, A.; Durand, E.; Feuga, B. and Peaudecerf, P. 1990 *Modeling fracture flow with a stochastic discrete fracture network: calibration and validation: 1. The flow model*. Water Resour. Res. 26, 479–489.
2. Dershowitz, W. S. and Fidelibus, C. 1999 *Derivation of equivalent pipe networks analogues for three-dimensional discrete fracture networks by the boundary element method*. Water Resource Res. 35, 2685–2691
3. Erhel, J.; de Dreuzy, J.-R. and Poirriez, B. 2009 *Flow Simulation in Three-Dimensional Discrete Fracture Networks*. SIAM J. Sci. Comput. 31, 2688–2705.
4. Vohralík, M.; Maryška, J. and Severýn, O. 2007 *Mixed and nonconforming finite element methods on a system of polygons*. Applied Numerical Mathematics 51, 176–193.
5. Berrone, S. and Scialò, S. 2011 *An Extended Finite Element Optimization Method For Simulating Discrete Fracture Network Flows*. tech. rep., Dipartimento di Matematica, Politecnico di Torino.

An immersed boundary method applied to cardiovascular simulations.

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Reduced models of fluid flows or mass transport in heterogeneous media are often used to save computational resources when the system to be simulated is too complex.

In this framework the immersed boundary method (IB) is proposed for the solution of complex fluid and deformable structure interaction problems encountered in many physical models [2], [3]. To avoid resolving the complex 3D geometry of the submerged structure we take into account only the 1D geometrical description of the structure centerline, defining a fiber network. The idea of this method is to define an asymptotic problem applying a suitable rescaling and replace the immersed interface and the related conditions by an equivalent mass source term.

This method is applied to the study of cardiovascular drug eluting stents deployed in coronary bifurcations. The problem involves the interaction of arterial deformations, hemodynamics and controlled drug release. Resorting to an immersed boundary method facilitates the handling of complex stent pattern and simplifies the definition of the mathematical model for drug release [1].

The method is also used in the context of modelling blood flow and drug transport through a network of capillaries surrounded by the porous interstitium of a solid tumor.

1. D'Angelo, C., Zunino, P., Porpora, A., Morlacchi, S., Migliavacca, F. 2011 *Model reduction strategies enable computational analysis of controlled drug release from cardiovascular stents*. SIAM Journal on Applied Mathematics, 71, 2312-2333.
2. Liu, W. K., Zhang, L., Gerstenberger, A., Wang, X., Liu, W. K. 2004 *Immersed finite element method*. Computer Methods in Applied Mechanics and Engineering, 193, 2051-2067.
3. Liu, W. K., Liu, Y., Farrell, D., Zhang, L., Wang, X. S., Fukui, Y., Patankar, N., Zhang, Y., Bajaj, C., Lee, J., et al. 2006 *Immersed finite element method and its applications to biological systems*. Computer Methods in Applied Mechanics and Engineering 195, 1722-1749.

MSP 42 - Optimization methods for inverse problems in imaging and machine learning

The mathematical models for inverse problems in imaging and machine learning applications are often formulated as large scale nonlinear programming (NLP) problems, whose objective functional is the combination of a fit-to-data term and a regularization term which mitigates the effect of the ill-posedness. The design of suited optimization methods is a challenging task not only for the large scale of these NLP problems, but also because in many applications the special features in the solution forced by the regularization term (e.g. sparsity, edge-preserving) can lead to solve nonsmooth optimization problems. In recent years, new optimization-based tools have been proposed to solve problems in imaging and machine learning applications, while these problems have led to deeper investigation and development of optimization algorithms. This minisymposium aims to strengthen the interaction between imaging, machine learning and optimization to discuss possible advances in these areas. Contributions to first and second-order methods, dual or primal-dual approaches and subgradient-type schemes will be considered for biomedical imaging applications.

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Nonparametric sparsity via derivative based regularization

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In this work we are interested in the problems of supervised learning and variable selection when the input-output dependence is described by a nonlinear function depending on a few variables. Our goal is to devise a sparse nonparametric model, and our work can be considered as a first step towards understanding the role of sparsity beyond additive models [1]. The key intuition is to measure the importance of each variable in the model by making use of partial derivatives. Based on this idea we propose and study a new regularizer and a corresponding least squares regularization scheme. Using concepts and results from the theory of reproducing kernel Hilbert spaces and proximal methods, we show that the proposed learning algorithm induces a minimization problem which can be provably solved by an iterative procedure. The consistency properties of the obtained estimator are studied both in terms of prediction and selection performance. An extensive empirical analysis shows that the proposed method performs favorably with respect to the state-of-the-art.

1. Mosci, S. and Rosasco, L. and Santoro, M. and Verri, A. and Villa, S., Nonparametric sparsity and regularization, <http://hdl.handle.net/1721.1/65964>, 2011

Optimized limited angle tomography

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Although cone-beam imaging is gaining more and more popularity also in the field of localized tomography, its high dose is often not justified in several applications, like breast tumor screening and dental implantology. In these domains, algebraic reconstruction techniques [1] and limited angle acquisition are being fully exploited as they are potentially able to convey all the information required to clinicians with a lower dose.

However, limited angle acquisition introduces what are called truncation and band artifacts that have an important impact on the final image quality.

We will describe the solutions proposed by our group. Truncation artifacts have been tackled by reformulating the tomographic problem in the context of weighted least-squares estimate to limit the impact of rays that intersect the reconstructed volume for a short length. Band artifacts can be eliminated reformulating the problem in the context of the regularization theory where homogeneity of the reconstructed volume is facilitated at the boundary of two projections.

We have also developed a parallel version of the modified algebraic reconstruction engine and implemented on a CUDA architecture. This implementation allows producing the tomography, starting from 11 projections, in less than 5s.

1. Kak, A. C. and Slaney, M. 2001 *Principles of Computerized Tomographic Imaging*. Classics in Applied Mathematics - SIAM.

An alternating direction method for constrained linear least-squares problems with application to image restoration

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The alternating direction method for convex programming is an implementable variant of the augmented Lagrangian multiplier method. Recently it has been successfully applied in image restoration with Tikhonov regularization and in Total Variation regularization. In this talk, an alternating direction method for solving constrained linear least-squares problems is presented and analyzed. The procedure requires at each iteration the solution of two subproblems: the first is a linear system, the second is a bound-constrained optimization problem with closed-form solution. Experimental results for image deblurring problems illustrate that the method is effective in terms of quality of the restored images and speed and compares favorably with alternative approaches.

Primal–dual hybrid gradient algorithms for image restoration

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In this study we establish the convergence of a general primal–dual method for nonsmooth convex optimization problems whose structure is typical in the imaging framework, as, for example, in the Total Variation image restoration. When the steplength parameters are *a priori* selected sequences, the convergence of the scheme is proved by showing that it can be considered as an ϵ -subgradient method [1,2] on the primal formulation of the variational problem. Our scheme includes as special case the method recently proposed in [3] for Total Variation image restoration from data degraded by Gaussian noise. Furthermore, the convergence hypotheses enable us to apply the same scheme also to other restoration problems, as the denoising and deblurring of images corrupted by Poisson noise, where the data fidelity function is defined as the generalized Kullback–Leibler divergence, or the edge preserving removal of impulse noise. The numerical experience shows that the proposed scheme with a suitable choice of the steplength sequences performs well with respect to state-of-the-art methods, especially for Poisson denoising problems, and it exhibits fast initial and asymptotic convergence.

1. Larsson, T., Patriksson, M. and Strömberg, A.B. 2003 *On the convergence of conditional ϵ -subgradient methods for convex programs and convex–concave saddle-point problems*. European Journal of Operational Research 151, 461–473.
2. Robinson, S.M. 1999 *Linear convergence of epsilon-subgradient descent methods for a class of convex functions*. Math. Program., Ser. A 86 1999, 41–50.
3. Zhu, M. and Chan, T.F. 2008 *An efficient primal–dual hybrid gradient algorithm for Total Variation image restoration*. CAM Report 08-34, UCLA.

MSP 043 - Packing optimization problems in space engineering

This mini-symposium originates from research carried out in space engineering, in support to the cargo accommodation. Usually the goal consists of maximizing the loaded mass/volume in compliance with given rules. Complex geometries have to be tackled, besides balancing conditions. Small items can be assumed to be parallelepipeds, but, generally, such approximation does not realistically hold when dealing with large items. Tetris-like items are, in most cases, more suitable, and similar considerations concern the container shape as well.

The literature on the packing optimization problems (NP-hard) is extensive, but most of the research focuses on the orthogonal placement of parallelepipeds inside parallelepipeds, with no additional conditions. When dealing with non-standard packing problems with overall conditions, such as balancing, a global optimization point of view becomes indispensable. The approach put forward focuses on mixed integer linear/non-linear programming and ad hoc heuristics.

The first presentation outlines the overall methodology adopted. The second looks upon the issue of exploiting the free volume of partially loaded containers by adding virtual items. A non-linear approach, aimed at looking into approximate solutions to the basic packing problem, is discussed by the third one. The fourth provides insights into the applicative context.

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A global optimization approach for solving non-standard packing problems with additional constraints

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This work originates from research carried out in support to the cargo accommodation of space vehicles/modules. The goal of this activity is to maximize the loaded cargo, taking into account the given accommodation requirements. Items can often be modelled as parallelepipeds, but it is even more frequent that real-world issues make this approximation no longer acceptable. These aspects and the presence of additional overall conditions, such as balancing, give rise to very challenging non-standard packing problems, not only in the frame of space engineering, but also in different application areas. The presentation considers first the orthogonal packing of tetris-like items, within a convex domain and subsequently the packing of polygons with (continuous) rotations in a convex domain. The proposed approach is based on mixed integer linear/non-linear programming (MIP, MINLP), from a global optimization (GO) point of view. The tetris-like formulation is exploited to provide the MINLP solution process with an approximated starting solution.

Exploiting empty spaces of a partially loaded container by adding virtual items

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This work originates from a research activity recently carried out by Thales Alenia Space, in support to the International Space Station logistics. It investigates the issue of adding a number of virtual items (i.e. items not given a priori) inside partially loaded containers, in order to exploit the volume still available on-board, as much as possible. Items already accommodated are supposed to be tetris-like-shaped, while the additional virtual ones are assumed to be parallelepipeds. A mixed integer non-linear programming (MINLP) model is introduced first, then possible linear approximations to it are discussed and a mixed-integer-linear-based (MIP) heuristic approach proposed. Guidelines for future research are pointed out and experimental insights are provided to show the efficiency of the adopted approach.

Approximate solutions to the basic 3D-packing MIP model by a non-linear Approach

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This work extends a previous research focused on a mixed integer programming (MIP) based heuristic approach, aimed at solving non-standard three-dimensional packing problems with additional constraints. The presentation looks upon a mixed integer non-linear (MINLP) reformulation of the basic (MIP) model, to improve the former heuristic, based on linear relaxation. The approach put forward is addressed, in particular, to standard MINLP solvers up to exploiting linear substructures of the mathematical model.

The CAST (Cargo Accommodation Support Tool) project

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The Automated Transfer Vehicle (ATV) is the European Space Agency (ESA) transportation system supporting the International Space Station (ISS). A detailed analytical cargo accommodation for each single cargo has to be performed in order to meet the Cargo Manifest plan provided by NASA. Demanding accommodation rules, geometrical and functional conditions have to be considered, in addition to the static and dynamic balancing constraints, deriving from the attitude control requirements. The objective of the analysis is to satisfy the Cargo Manifest, in compliance with the given accommodation rules and constraints. The problem is very challenging and looking into an efficient solution, by means of a manual approach alone, would represent an impractical job even for an experienced designer. CAST has been funded for this purpose by ESA. An ad hoc tool version, tailored to the Columbus (ISS attached laboratory) stowage problem, has been further implemented and is going to be used from now on.

MSP 44 - Topics in classical mechanics

The minisymposium collects recent advances in theoretical and applied mechanics. Talks will deal with new analytical and numerical methods for classical problems, as well as with mathematical modeling of complex phenomena (like chemical reactions), based on classical mechanics.

Organizer:

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A unified master-equations-based setting for the analysis of chemical reactions

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An important research topic in the field of Systems Biology is the detection of efficient methods for modeling complex cellular mechanisms. Recently it has been pointed out the importance of the noise role in the dynamics of biological processes. Generally speaking, the role of stochastic fluctuations is particularly important in the dynamics of biochemical reactions in which are involved a low number of molecules. These assumptions lead to the statement that the time-evolution of the number of copies of the involved players is well described by the probabilistic approach given by the so-called Chemical Master Equations (CME).

For a general set of chemical reactions a multi-dimensional Markov-chain model is written, describing the molecular behavior of all the chemical species therein involved. The related multi-dimensional CME model, describing the time-evolution of the probabilistic concentrations for any species, is then derived. Some structural properties of the CME model are pointed out, allowing a computationally cheap management of some classical analytic tasks such as the determination of the equilibrium distributions and the simulation of the underlying stochastic processes related to the molecular behavior of the whole chemical reaction.

An ES-BGK model for a reacting gas mixture

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A relaxation-time-approximation of a simple Boltzmann kinetic model for a slow bimolecular chemical reaction is presented. The dominant elastic operator is approximated by an ellipsoidal BGK-operator recently proposed in the literature [3] which ensures correct constitutive equations for the diffusion velocities of the inert gas. The hydrodynamic limit up to the fluid-dynamic reactive Navier-Stokes equations is worked out by a Chapman-Enskog asymptotic procedure. Results indicate that transport coefficients are not affected by the slow reaction, but reactive effects are described by additional source terms, vanishing at chemical equilibrium, appearing in the non-conservative balance equations for species densities and for temperature. Results are in agreement with similar kinetic results on slow chemical reactions [2], and at variance with the fast chemical scenario, in which source terms are absent, and reaction does affect instead transport coefficients, and also introduces an additional scalar pressure [1].

1. Bisi, M., Groppi, M. and Spiga, G. 2010 *Kinetic Bhatnagar-Gross-Krook model for fast reactive mixtures and its hydrodynamic limit*. Phys. Rev. E 81, 036327.
2. Bisi, M. and Spiga, G. 2011 *On a kinetic BGK model for slow chemical reactions*. Kin. Relat. Mod. 4, 153–167.
3. Brull, S., Pavan, V. and Schneider, J. 2012 *Derivation of a BGK model for mixtures*. Eur. J. Mech. B-Fluids 33, 74–86.

Exponentially fitted methods for second order ordinary differential equations with parameter estimation

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In this talk we deal with exponentially fitted methods for the numerical solution of second order ordinary differential equations of type $y'' = f(x, y)$, whose solutions are known to show a prominent exponential behaviour depending on the value of one or two unknown parameters to be suitably determined. The knowledge of an estimation to the unknown parameters is needed in order to apply the numerical method, since its coefficients depend on the value of such parameters. We construct a new exponentially fitted method and present a strategy for the practical estimation of the parameters.

1. Ixaru, L. Gr. and Vanden Berghe G. 2004 *Exponential fitting*, Kluwer Academic Publishers, Dordrecht.
2. D'Ambrosio, R., Ferro, M. and Paternoster B. 2009, *Two-step hybrid collocation methods for $y'' = f(x, y)$* , Appl. Math. Lett. 22, 1076-1080.
3. D'Ambrosio, R., Ferro, M. and Paternoster B. 2011, *Trigonometrically fitted two-step hybrid methods for second order ordinary differential equations with one or two frequencies*, Math. Comput. Simul. 81, 1068-1084.

Metereological fractional models of pollution based on anomalous diffusion

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During the past years, the subject of fractional calculus has gained considerable popularity and importance mainly due to its demonstrate applications in numerous diverse widespread fields in science. A number of possible numerical methods for solving the time , or space, or time-space fractional anomalous diffusion have been proposed [1] [2] [3] [4] [5] [6]. The dominant numerical methods for solving fractional partial differential equations are based on the finite difference method, finite element method, finite volume method, meshfree method and the matrix tranform method. Numerical methods are proposed for solving two-dimensional partail differential equarions. Will be used the fractional Caputo derivative in time, and the fracional Laplacian operator will be defined through the eigenfunction expansion on a finite domain. The error bounds for the numerical schemes and the analytical solution are also derived. Numerical experimets are carried out to assess the computational performance and accuracy of our scheme, and some conclusions are drawn. Finally are proposed some extentions with respect to what avalaible in the present literature.

1. Chang-Ming Chen, F. Liu, I. Turner, 2007, A Fourier method for the fractiona diffusion equation describing sub-diffusion *Journal of Computaional Physics*. Page In Press.
2. R. Lin, F. Liu, V. Anh, and I. Turner, 2009, Stability and convergence of a new explicit finite-difference approximation for the variable-order nonlinear fractional diffusion equation *Applied and Computational Mathematics*. . 212(2):435-445.
3. Q. Yang,2010, Novel analytical and numerical methods for solving fractional dynamical systems *Thesis for the degree of a Doctor of Philosophy in the Faculty of Sciance and Technology*.
4. Q. Yang, F. Liu, and I. Turner 2010, Stability and convergence of an effective numerical method for the time-space fractional Fokker-Planck equation with a nonlinear source term *International Journal of differential equations*. Article ID 464321.
5. H. Zhang, F. Liu, and V. Anh, 2007, Numerical approximation of Lévy-Feller diffusion equation and its probability interpretation *Journal of Computational and Applied Mathematics*. 206(2): 1098-1115.
6. P. Zhuang, F. Liu,V. Anh, and I. Turner 2009, Stability and convergence of an implicit numerical method for the nonlinear fractional reaction-subdiffusion process *IMA Journal of Applied Mathematics*. 74): 645-667.

MSP 45-46 - Topics in fluid dynamics I - II

In this mini-symposium people involved in many fields of fluid dynamics are gathered to present a survey of recent progress of their work.

Several models and methodologies are proposed in these two sessions, and they all deal with problems arising in the frame of the most diverse fluid dynamic applications. In fact, they are concerned with fluids of different nature, as well as flows of different features, driven by different forces and confined by geometrical constraints of different physical — and, sometimes, topological — dimensions.

Corresponding to this variety of challenging problems, a number of tools is involved: some appear more dedicated, due to the compelling role of specific conditions, some exhibit potential for wider applicability. Many are based on a careful combination of theoretical modeling and efficient computational treatment.

Common origin of these contributions is the intrinsic, deep mathematical content that is revealed in all the folds of the fluid dynamic phenomena.

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MHD three-dimensional stagnation-point flow of a Newtonian and a micropolar fluid

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The steady three-dimensional stagnation-point flow of an electrically conducting Newtonian or micropolar fluid in the presence of a uniform external magnetic field \mathbf{H}_0 is analyzed and some physical situations are examined.

In particular, in [1] it has been proved that, if we impress an external magnetic field \mathbf{H}_0 , and we neglect the induced magnetic field, then the steady three-dimensional MHD stagnation-point flow is possible if, and only if, \mathbf{H}_0 has three particular directions.

In all cases it is shown that the governing nonlinear partial differential equations admit similarity solutions. I will show that for the three situations the flow of a Newtonian or a micropolar has to satisfy an ordinary differential problem whose solution depends on \mathbf{H}_0 through the Hartmann number M^2 .

Finally, thanks to the numerical integration, I will show the behaviour of the solutions and I will underline some interesting aspects that come out for the presence of the magnetic field.

1. Borrelli, A., Giancesio, G., Patria, M.C. 2011 *MHD three-dimensional stagnation-point flow of a Newtonian and a micropolar fluid*. IJPAM 73, 2, 165–188.

A mathematical and numerical model for explosive volcanic eruptions

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We propose a mathematical and numerical model for explosive volcanic eruptions that allows to describe pyroclastic flows both in supersonic and subsonic regimes taking into account dust particles of non uniform grain size. The semi-implicit numerical method includes second order time and space discretizations and fully multidimensional advection schemes [1] [2]. Time dependent vent conditions are also considered, in contrast to the constant vent conditions employed in the models described in the literature [3][4]. The method has been implemented in a parallel code that allows for realistic simulations. Numerical experiments in two and three dimensions show that the resulting technique is efficient and accurate and significantly improves several aspects of the simulation of pyroclastic flows with respect to the models described in the literature.

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- [2] LeVeque, R.J., High-resolution conservative algorithms for advection in incompressible flow, *SIAM Journal of Numerical Analysis*, **33** (1996) pp. 627-665
- [3] Neri, A., Esposti Ongaro, T., Macedonio, G. and Gidaspow, D., Multiparticle simulation of collapsing volcanic columns and pyroclastic flow, *Journal of Geophysical Research*, **108** (2003) pp. 2002-2015
- [4] Pelanti, M. and LeVeque, R.J., High-resolution finite volume methods for dusty gas jets and plumes, *SIAM Journal of Scientific Computing*, **28** (2006) pp. 1335-1360

Droplets spreading under contact-line friction

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This talk is concerned with the spreading of a liquid droplet on a plane solid surface in the regime of lubrication approximation. The focus is on effective conditions which relate the speed of the contact line (where liquid, solid and vapor meet) to the microscopic contact angle. One such condition has been recently proposed by Weiqing Ren and Weinan E [1]: it includes into the model the effect of frictional forces which arise at the contact line from unbalanced components of the Young's stress, leading to an additional dissipation term in the energy balance. For speed-dependent contact angle conditions of rather general form, a matched asymptotic study is worked out, relating the macroscopic contact angle to the speed of the contact line. Here, well-posedness for a class of traveling-wave solutions, which does not seem to have been observed so far, is proved and used. For the specific model of Ren and E, ODE arguments are then applied to infer the intermediate scaling laws and their timescales of validity: in complete wetting, they depend crucially on the relative strength of surface friction (at the liquid-solid interface) versus contact-line friction; in partial wetting, they also depend on the magnitude of the static contact-angle.

1. Ren, E and E, W. 2007 *Boundary conditions for the moving contact line problem*. Phys. Fluids 19, 022101.

Stokes flows in axisymmetric geometries

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Enrico De Bernardis

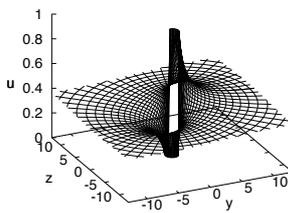
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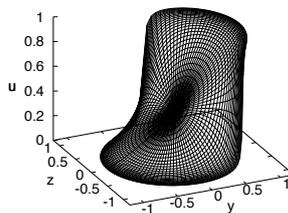
In planar geometries the extended Stokes' problems for a Newtonian fluid lead to well known solutions [1,2]. The present talk is aimed to perform the same calculations, but in a cylindrical geometry.

The Stokes flows outside or inside a circular cylinder are analytically solved. The cylinder rotates around or translates along its axis (named as x) with a time (t) dependent velocity: $U(t) = U_0 H(t)$ (first problem) or $U(t) = U_0 H(t) \cos(\omega t + \varphi)$ (second), $H(t)$ being 1 as $t > 0$ and 0 as $t < 0$. The *extended* problems are also investigated. They are generated by the rotation of only half cylinder (*e.g.* the one having $x > 0$), or by the translation of only the part of the cylinder belonging to a dihedral angle (α, β) having its edge on x . The first problem is called *extended tangential* one, while the second problem *extended axial* one. Mathematical details about their solutions will be given in the talk.

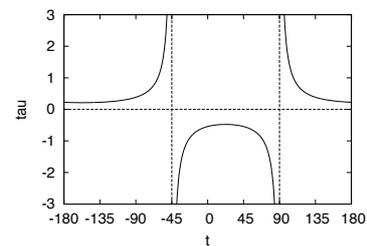
In figure, the nondimensional axial velocity \tilde{u} (U_0 is used as a reference velocity) at large times for the extended axial ($\alpha = -\pi/4$, $\beta = +\pi/2$) first problem outside (a) and inside (b) the cylinder are drawn vs. the nondimensional coordinates \tilde{y} , \tilde{z} (the radius R of the cylinder is used as reference length). Note that the velocity goes to $(\beta - \alpha)/(2\pi)$ at large distances from the cylinder. In (c) the nondimensional wall stress $\tilde{\tau}$ (the stress divided by $\mu U_0/R$, μ being the coefficient of viscosity of the fluid) at large times is drawn vs. the angular coordinate θ . As expected, the stress diverges in correspondence to the values α and β of θ .



(a)



(b)



(c)

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2. Riccardi, G. 2011 Remarks on the solution of extended Stokes' problems. Int. J. of Non-linear Mechanics, vol. 46-7, pp 958-970.

Spectral gaps for water waves above a corrugated bottom

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We consider a layer of an incompressible inviscid liquid above a periodically corrugated surface. We deal with the time-harmonic waves standing at or travelling along a submerged body. Under certain geometric conditions the essential spectrum of the corresponding boundary value problem has gaps, whose position and length can be found by applying an asymptotic analysis to the model problem in the periodicity cell.

An Eulerian-Lagrangian approach for interface tracking in free boundary problems

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In the numerical modelling of free surface flows, like those occurring at the sea surface due to the air-water interaction, the interface is either tracked by Lagrangian approaches or captured in the computational domain through suitable functions. Lagrangian tracking is generally rather accurate and characterized by good conservation properties, but it makes it challenging dealing with topological changes. Interface capturing methods are much simpler on this respect but, as a drawback, they induce large errors in terms of mass conservation properties.

An Eulerian-Lagrangian algorithm for free surface flows is developed. A set of material particles are distributed on the free surface and are advected in a Lagrangian way. The signed distance from the free surface is then reinitialized on a subgrid which has, say, 4x4 subcells in each cell of the computational grid. A bilinear interpolation of the distance on the subcell system is used to reconstruct the set of segments representing the new interface configuration. Preliminary results indicate that an improvement of the conservation properties and a reduction of the computing times are achieved compared to the pure level set method.

MSP 47 - Topics in rational mechanics

This minisymposium is devoted to some special topics arising in mechanics. It consists in three individual talks. The first one concerns a model for elastic wires which takes into account the heat conduction and makes use of methods of extended thermodynamics. The second contribution is devoted to present a new nonlinear model to describe the motion of a two-mass skate bicycle, recently developed as a simplified bicycle. Finally the last talk concerns the modeling and the control of a small helicopter called mikrokopter. The dynamics of such a helicopter is derived from both the Newton-Euler equations and the Euler-Lagrange equations.

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Mathematical modeling of mikrokofter

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Mikrokofter is a small helicopter which has become increasingly popular as Unmanned Aerial Vehicle (UAV) platforms. Due to the specific capabilities, the employment of mikrokofter has become very popular, it is used for surveillance, search and rescue.

In order to develop proper methods for the stabilization and the trajectory control of the mikrokofter is necessary to build an appropriate mathematical model. The purpose of this talk is to present the basics of mikrokofter modeling and control.

The mikrokofter we take into account consists of six rotors in total, with three pairs of counter-rotating, fixed-pitch blades, two of them are located at the four corners, and the third is on the top of the aircraft. The mikrokofter is controlled by adjusting the angular velocities of the rotors which are spun by electric motors. The differential equations of the mikrokofter dynamics are derived from both the Newton-Euler equations and the Euler-Lagrange equations.

1. G.M. Hoffmann, H. Huang, S.L. Waslander and C.J. Tomlin, 2007 Quadrotor helicopter flight dynamics and control: Theory and experiment. In *Proceedings of the AIAA Guidance, Navigation and Control Conference and Exhibit*. American Institute of Aeronautics and Astronautics, Inc..
2. G.M. Hoffmann, H. Huang, S.L. Waslander and C.J. Tomlin, 2009 Aerodynamics and control of autonomous quadrotor helicopters in aggressive maneuvering. In *IEEE International Conference of Robotics and Automation*. 3277–3282.

Nonlinear analysis of the two-mass-skate bicycle model

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A simplified bicycle model, called two-mass skate (TMS), has been recently developed by Kooijmann et al. [2] for studying the self-stability of a bicycle which is not affected by neither gyroscopic nor caster effects, usually related with the real motion of such a system.

Numerical analyses and a wide series of experiments have pointed up that the TMS can automatically steer itself so as to recover from falls. These results are obtained by using the model introduced by Whipple (in 1899) characterized by 25 parameters, which in this case are reduced to a more manageable 8, and linearizing the equations of motion for small perturbations of the upright steady forward motion.

In this paper we revise the kinematics of the TMS model and we derive the nonlinear equations of motion for the system, taking the nonholonomic constraints on the velocities into account, from a geometric point of view [1]. Furthermore, studying the behaviour of this system, we analyze its stability, which exhibits some peculiar aspects due to the nonholonomy of the problem.

1. Bloch, A. M. (with the collaboration of J.Baillieul, P.Crouch, and J.Marsden) 2003 *Nonholonomic mechanics and control*. New York, Springer.
2. Kooijmann, J. D. G. et al. 2011 *A bicycle can be self-stable without gyroscopic or caster effects*. Science 332, 339–342.

MSP 048 - Quasi-variational inequalities, generalized Nash equilibrium problems and applications

Recently, there has been a sharp increase in interest in modelling generalized Nash equilibrium problems in order to represent real-life situations, such as oligopoly models, environmental problems, network problems, infrastructure problems and electric power supply problems. The aim of this minisymposium is to bring together scholars working on both theoretical and computational issues, present results having potential of solving concrete problems, and thus try to fill the gap between theory and practice.

The approach chosen for dealing with such challenging problems is based on quasi-variational inequalities in both finite and infinite dimensional spaces, that are naturally associated to generalized Nash equilibrium problems. Four applications are proposed:

1. Market incompleteness generated by Market Coupling, the most advanced market design in the restructured European electricity system.
2. Effects of EU-ETS directives on the cement industry with a particular focus on the Italian market, the second European cement producer.
3. Power allocation chosen by radio resources in order to obtain satisfying quality signals avoiding interferences.
4. Optimal investment allocation in environmental projects within Kyoto Protocol commitments.

Topics of interest include, but are not limited to: quasi-variational inequalities, generalized Nash equilibrium, computation, approximation and algorithms, European electricity system, cement industry, radio resources, climate change.

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Quasi-variational inequalities, generalized Nash equilibrium and market coupling imperfections

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“Market Coupling” is currently seen as the most advanced market design in the restructuring of the European electricity market. Market Coupling, by construction, introduces what is generally referred to as an incomplete market: it leaves several constraints out of the market and hence avoids pricing them. This may or may not have important consequences in practice depending on the case on hand. Quasi-Variational Inequality problems and the associated Generalized Nash Equilibrium [1], [2], [3], [5], [7], [9] can be used for representing incomplete markets. Recent papers [4], [6], [8], [10] propose methods for finding a set of solutions of Quasi-Variational Inequality problems. We apply one [10] of these methods to a subproblem of Market Coupling, namely the coordination of counter-trading. We first discuss the economic interpretation of the Quasi-Variational Inequality problem. We then apply the algorithmic approach to a set of stylized case studies in order to illustrate the impact of different organizations of counter-trading.

1. Facchinei, F. and Pang, J. S. 2003 *Finite-dimensional variational inequalities and complementarity problems*, vols 1 and 2. Springer.
2. Facchinei, F. and Pang, J. S. 2010 Nash equilibria: the variational approach. In *Convex optimization in signal processing and communications* (ed. Palomar, D. P. and Y. C. Eldar), pp. 443–493. Cambridge University Press.
3. Facchinei, F. and Kanzow, C. 2007 *Generalized Nash equilibrium problems*. 4OR, 5, 173–210.
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10. Nabetani, K., Tseng, P. and Fukushima, M. 2009 *Parametrized variational inequality approaches to generalized Nash equilibrium problems with shared constraints*. Comput. Optim. Appl. 48(3), 423–452.

The cement sectors carbon leakage: a generalized Nash equilibrium problem

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This paper presents a non-linear Generalized Nash Equilibrium Problem to investigate the effects of EU-ETS Directives on the cement industry with a particular focus on the Italian market, the second European cement producer. This model is able to represent the interaction of cement companies that maximize their profit simultaneously since their strategies are interrelated by the market clearing conditions, common to all the companies. Quasi-Variational Inequality problems and the associated Generalized Nash Equilibrium [1], [2], [3], [5], [6] can be used for representing these markets. We adopt a technological representation of the market to have a direct control of the different sources of cost (energy, raw materials, CO₂ allowances and transportation) and the factors that may induce companies to displace their emissions (the carbon leakage effect). In this analysis, a key role is played by transportation costs that are particularly high in this sector.

1. Facchinei, F. and Pang, J. S. 2003 *Finite-dimensional variational inequalities and complementarity problems*, vols 1 and 2. Springer.
2. Facchinei, F. and Pang, J. S. 2010 Nash equilibria: the variational approach. In *Convex optimization in signal processing and communications* (ed. Palomar, D. P. and Y. C. Eldar), pp. 443–493. Cambridge University Press.
3. Facchinei, F. and Kanzow, C. 2007 *Generalized Nash equilibrium problems*. 4OR, 5, 173–210.
4. Facchinei, F. and Sagratella, S. 2010 *On the computation of all solutions of jointly convex generalized Nash equilibrium problems*. Optim Lett. 5(3), 531–547.
5. Facchinei, F., Fischer, A. and Piccialli, V. 2007 *On generalized Nash games and variational inequalities*. Oper. Res. Lett. 35, 159–164.
6. Harker, P. T. 1991 *Generalized Nash games and quasi-variational inequalities*. Eur. J. Oper. Res. 54, 81–94.

Nash equilibrium existence for a cognitive radio power allocation model

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The radio spectrum is a finite resource whose occupancy and use are governed by complex national and international rules. The traditional fixed spectrum assignment policy is becoming inefficient: the increasing demand of radio resources, like mobile phones and Internet service, is making some frequency bands of the radio spectrum more and more crowded with users interfering the ones with the others.

A Cognitive Radio system, where radios are able to change their transmitter parameters (like frequency or signal power) basing on the interaction with the environment in which they operates, is promising in order to obtain a more efficient spectrum use.

Game Theory is appropriate to analyse the problem of power allocation chosen by radio resources in order to obtain a satisfying quality signal avoiding an excessive interference to the other users.

A recent energy-efficient model for a Cognitive Radio scenario with primary and secondary users is here analysed in order to obtain conditions ensuring the existence of a Nash Equilibrium for the proposed Game in a continuous-time scenario.

A quasi-variational inequality approach to environmental projects

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We show how one of the Kyoto Protocol mechanisms, the so-called joint implementation in environmental projects (see [1]), can be transformed into and studied as an infinite dimensional quasi-variational inequality. Specifically, we examine the situation in which different countries, aiming at fulfilling Kyoto Protocol commitments, seek to determine the optimal investment allocation in environmental projects and the tolerable pollutant emissions, so as to maximize their welfare. We state the equilibrium conditions governing the model (see [2], [3]) and provide an equivalent quasi-variational formulation. Finally, we discuss the existence of solutions.

1. Breton, M., Zaccour, G. and Zahaf, M. 2006 *A game-theoretic formulation of joint implementation of environmental projects*. European J. Oper. Res. 168, 221-239.
2. Scrimali, L. 2010 *A variational inequality formulation of the environmental pollution control problem*. Optim. Lett. 4 (2), 259-274.
3. Scrimali, L. 2012 *Pollution control quasi-equilibrium problems with joint implementation of environmental projects*. Appl. Math. Letters 25, 385-392.

MSP 49 - Variational inequalities and network equilibrium problems

The Minisymposium deals with one of the most important research fields of Mathematics, namely Variational Inequalities and Equilibrium Problems, especially those related to network design.

Variational Inequalities proved to be a very useful and powerful tool for investigation of solutions of many equilibrium problems in Economics, Engineering, Operations Research and Mathematical Physics. They provide, as a matter of fact, a unifying framework for the study of diverse problems as boundary value problems, price equilibrium and traffic network equilibrium problems, Walras problem, vaccination problem, oligopolistic market equilibrium problem, financial problem. In particular, when considering the above problems in their evolution in time they are modelled by evolutionary variational inequalities. Several classical and new theories, such as those of Evolutionary Projected Dynamical Systems and Infinite Dimensional Duality, as well as research in discretized computational methods, have received a decisive impulse in order to offer effective solutions to hitherto unsolved problems. For this reason, particular emphasis will be given to the development of the Variational Inequalities Theory as for example the research of regularity results and their use to the computational procedure.

Therefore, the Minisymposium aims to offer a review of research themes, methods and open problems together with outlines of the new research trends in all the above topics.

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Advanced results on infinite dimensional duality in elastic-plastic torsion

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The aim of the talk is to present very recent results on the existence of Lagrange multipliers associated to the elastic-plastic torsion problem. More precisely we present the result of existence of a Radon measure, which plays the role of a Lagrange multiplier for the elastic-plastic torsion problem. Then, we recall the new strong duality theory introduced in [1] and the applications, contained in [2], of this theory to the Lagrange multipliers associated to the elastic-plastic torsion problem and finally we provide some consequences (see [3]).

1. Daniele, P., Giuffrè, S., Idone, G. and Maugeri, A. 2007 *Infinite Dimensional Duality and Applications*. Math. Ann. 339, 221-239.
2. Daniele, P., Giuffrè, S., Maugeri, A. and Raciti, F. *Duality theory and applications to unilateral problems*. Submitted.
3. Giuffrè, S. and Maugeri, A. *New results on infinite dimensional duality in elastic-plastic torsion*. Accepted on FILOMAT.

Partial cooperative games

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In this paper I study an approach through partial cooperative models to environmental problems via mathematical Game Theory. In general not all players wish to cooperate to solve a common problem (for example a pollution problem) so I consider a model with n players but only some of them wish to cooperate. Keeping into account the theory of cooperative games and the theory of non cooperative ones a coalition game is transformed into a strategic one and I use the solution concept for partial cooperative games as introduced in [7].

I consider multicriteria games (or multiobjective games), in fact in the applications to reality a decision maker has not one but more objectives "to optimize" and often not comparable. I study the existence of coalitional Pareto equilibria for partial cooperative games.

Many examples complete the paper.

Key-words: cooperative games, non cooperative games, strong Nash solution, equilibrium problems.

1. Göran-Maler K., Xepapadeas A., De Zeeuw A., 2003 *The Economics of Shallow Lakes*, Environmental and Resource Economics, 26, 603-624.
2. Finus M., 2001 *Game Theory and International Environmental Cooperation* Edward Elgar ed..
3. Fläm S.D., 2006 *Balanced environmental games*, Computers and Operations Research, 33, 401-408.
4. Meca-Martínez A., Sánchez Soriano J., García-Jurado I., Tijs S., 1998 *Strong equilibria in claim games corresponding to convex games*. Int. Journal of Game Theory, 27, 211-217.
5. Myerson R., 1997 *Game Theory. Analysis of Conflict* Harvard University Press.
6. Patrone F., Pusillo L., Tijs S., 2007 *Multicriteria games and Potentials* TOP, 15, 138-145.
7. Pieri G., Pusillo L., 2012 *A partial cooperative approach to environmental problems*, submitted.
8. Pusillo L., Tijs S., 2012 *E-equilibria for Multicriteria Games* to appear in Annals of the International Society of Dynamic Games.

Partial cooperation in strategic games

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We consider an n -person strategic game where a group of players forms a coalition (signatories) and maximizes the aggregate welfare function. The other players (non-signatories) do not cooperate and choose a Nash equilibrium maximizing their own payoff. This scheme corresponds to a partial cooperative situation deeply used in IEA (International Environmental Agreements) contexts ([1]). We may assume that signatories and non-signatories choose their decision in the same time (Nash-Cournot assumption) or we may assume the leadership of the signatory group in a two-stage model (Stackelberg assumption). The partial cooperative equilibrium under Stackelberg assumption has been studied for special classes of games, namely potential ([2]) and aggregative games ([3]). The aggregative structure in the second case allowed to consider the possibility of non-signatories multiple decisions. The results have been applied to global emission games, public goods games, Cournot games. We investigate the partial cooperation under the Nash-Cournot assumption as well the Stackelberg one and discuss some properties in both situations, particularly the comparison of players profit.

1. Finus, M. 2001 *Game theory and international environment cooperation*. Edward Elgar Publishing.
2. Mallozzi, L. and S. Tijs 2008 *Conflict and cooperation in symmetric potential games*. Int. Game Theory Rev. 10, 1-12.
3. Mallozzi, L. and S. Tijs 2009 *Coordinating choice in partial cooperative equilibrium*. Econ. Bulletin 29, 1467-1473.

Retarded weighted quasi-variational inequalities for transportation problems

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The aim of the talk is to consider user equilibrium problems in transportation networks in the most complete and realistic situations. In fact, the presented model allows for the dependence of data on time, the presence of elastic travel demands, the capacity restrictions and delay effects. Moreover, the weights allow us to study the problem in the presence of congestion. The equilibrium conditions for such a model are given and the equivalent formulation in terms of a weighted quasi-variational inequality is discussed. Then, a theorem for the existence of solutions is shown. Moreover, by using the set convergence in Kuratowski's sense, a continuity result for equilibrium solutions is obtained. At last, a numerical example is provided.

1. Barbagallo, A. 2012 *Retarded weighted quasi-variational inequalities for traffic network equilibrium problems*, Optim. Eng., DOI 10.1007/s11081-011-9182-y.

**MSP 50-51 - Variational methods for problems in applied
sciences
I - II**

These minisymposia will put together researchers inspired by different problems in applied sciences, who share as a common background the methods and the techniques of the calculus of variations. Problems related to continuum mechanics and structures, material sciences will be considered by researchers in the fields of mathematics and engineering. In particular the first session will be focused on dislocations, interfacial energies arising in the framework of structured deformations. Nonlinear discrete scheme depending on second-order finite differences will be described for modelling image reconstruction, homogenization of nano structures, such as graphene sheet will be also presented. In the second session there will be a description of problems concerning random anisotropy properties in polycrystalline magnetic materials, multiple scale energies of biological membranes, polycrystal plasticity, evolution models for damage and for perfectly plastic plates.

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Asymptotic analysis of a system of edge dislocations

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We analyze a variational problem with topological singularities arising from the analysis of the elastic energy associated to a system of edge dislocations. We consider the core radius approach in which a neighborhood of the singularities of the strain field, corresponding to the dislocations, is removed and we study the asymptotic of the elastic energy outside the core in terms of Gamma-convergence in the logarithmic regime. This continuum model can be justified by an asymptotic analysis starting from a discrete description of dislocations (as in [3]) The analysis presents many similarities with the study of vortices in superconductivity via the Ginzburg-Landau energy, but also some specific difficulties due to the vectorial nature of the problem (see also [1]).

1. Alicandro R., Cicalese M., Ponsiglione M. 2011 *Variational equivalence between Ginzburg-Landau, XY spin systems and screw dislocations energies*. Indiana Univ. Math. J. 60, 171–208.
2. De Luca, L., Garroni, A. and Ponsiglione, M. 2012 *Γ -convergence analysis of systems of edge dislocations: the self energy regime*. ARMA, to appear.
3. Ponsiglione M. 2007 *Elastic energy stored in a crystal induced by screw dislocations: from discrete to continuous*. SIAM J. Math. Anal. 39, 449–469

An explicit formula for a relaxed interfacial energy arising from structured deformations

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The need in continuum mechanics to deal with multiscale geometrical changes has led Del Piero and Owen [1] to develop the concept of structured deformations. Successively, Choksi and Fonseca [2], starting from the energy associated to “simple” deformations, gave a definition of the energy of a structured deformation and deduced a representation theorem for such an energy.

Here we consider an energy density associated to a “simple” deformation with bulk energy density zero and with interfacial energy having a particular form. In this setting, and using the representation formula of Choksi and Fonseca, we deduce explicit formulas for the corresponding bulk and interfacial energies for structured deformations. Our result can be used to characterize how much, at a smaller length scale, pieces of a body are separating from one another and how much they are switching positions with one another.

1. Del Piero, G. and Owen, D. 1993 *Structured deformations of continua*. Arch. Rational Mech. Anal. 124, 99–155.
2. Choksi, R. and Fonseca, I. 1997 *Bulk and interfacial energy densities for structured deformations of continua*. Arch. Rational Mech. Anal. 138, 37–103.

Variational discrete models in image reconstruction

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We analyze a nonlinear discrete scheme depending on second-order finite differences. This is the two-dimensional analog of a scheme which in one dimension approximates a free-discontinuity energy proposed, in the framework of image processing, by Blake and Zisserman as a higher-order correction of the Mumford and Shah functional. In two dimensions we give a compactness result showing that the continuous problem approximating this difference scheme is still defined on special functions with bounded hessian, and we give an upper and a lower bound in terms of the Blake and Zisserman energy. We prove a sharp bound by exhibiting the discrete-to-continuous Γ -limit for a special class of functions, showing the appearance of new shear terms in the energy, which are a genuinely two-dimensional effect.

1. Braides, A. and Defranceschi, A. and Vitali, E. 2012 *A compactness result for a second-order variational discrete model* Mathematical Modelling and Numerical Analysis 46, 389–410

Homogenization of a graphene sheet

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Nano-materials are distinguished examples of micro structured media that stand at the forefront of modern materials science. Their discovery is the consequence of the enormous progress in the field of microscopy and of the refined techniques by which it is today possible to represent measure and manipulate matter practically at the atomic level. Graphene is a mono layer distribution of carbon atoms placed at the vertices of a hexagonal lattice and bonded by interatomic forces of mainly covalent type. Since the free edges are sites of high concentration of energy, in nature the sheets organize themselves in the form of single- or multi-layer cylinders in order to reduce the extent of free edges, thus giving rise to the so-called nanotubes.

By virtue of the strength of the bonds, these nano-structures have remarkable mechanical properties that make them very attractive for applications in various fields. On the other hand, their mechanical modelization is not yet firmly established for several reasons. First, the difficulty of managing the experimental measures, for which the availability of a sound theoretical framework would be of essence in setting up, performing and interpreting the tests. Second, the computational power which is still too limited to take full advantage of Molecular Dynamics approaches. These drawbacks have led researchers to resort to continuum models, which can be treated numerically and in some instances also analytically.

For nanotubes this has been done, for example, in [1]. But continuum models built in this way require information relating constitutive constants, such as the thickness of a monolayer or its bending stiffness, to molecular parameters, in ways which are difficult to define univocally and unambiguously for the discrete system.

As a first step towards the more challenging task to build up a continuum model for nanotubes, here I consider the case of graphene. I address the passage from discrete to continuum by using the general setting of Γ -convergence. In particular, I adapt the approach of [2, 3] for honeycomb cellular solids and get the equilibrium equations and the constitutive equations of the effective continuum. It is shown that the continuum problem is described by two vector fields - the macroscopic displacement and a corrugation vector field, the limit energy density depends upon. It turns out that the latter is implicitly determined by the strain components via auxiliary equilibrium equations. By taking this into account, the explicit form of the constitutive equations for the stress components is deduced.

1. Bajaj C., Favata A., Podio Guidugli P., On a nano-informed continuum-mechanical model of single-wall nanotubes, (2012), submitted.
2. Davini, C. and Ongaro, F., A homogenized model for honeycomb cellular materials, *J. Elasticity* **104** (1-2) (2011), 205-226.
3. Homogenization of linearly elastic honeycomb, *Mathematics and Mechanics of Solids*, (2012) (in print).

A multiple scales model for biomembranes and variational limits

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In a recent paper by Peletier and Röger [2] a variational model for the mechanical behavior of biomembranes is investigated at different scales. The passage from the microscopic proposed model to the mesoscopic scale is a simple argument, but it is much harder to recover a macroscopic model from the mesoscopic one. In [2] a full Γ -convergence result is proved in the 2D case: as limit one obtains a functional depending on the curvature, which is well known in literature as *Willmore functional*. In this talk I will present the work, still in progress, about the 3D case [1]: this is a joint work with M. Röger. The passage from 2D to 3D generates several new problems and very sophisticated tools coming from geometric measure theory are necessary, as for instance the theory of *generalized Gauss graphs*, which permits us to speak about curvature also for surfaces which are not regular.

1. Lussardi, L. and Röger, M. *Analysis of a variational model for the shape of biomembranes*. In preparation.
2. Peletier, M. and Röger, M. 2009 *Partial Localization, Lipid Bilayers, and the Elastica Functional*. Arch. Rational Mech. Anal. 193, 475–537.

A quasistatic evolution model for perfectly plastic plates derived by Γ -convergence

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The subject of this seminar is the rigorous derivation of a quasistatic evolution model for a linearly elastic - perfectly plastic thin plate. As the thickness of the plate tends to zero, we prove via Γ -convergence techniques that solutions to the three-dimensional quasistatic evolution problem of Prandtl-Reuss elastoplasticity converge to a quasistatic evolution of a suitable reduced model. In this limiting model the admissible displacements are of Kirchhoff-Love type and the stretching and bending components of the stress are coupled through a plastic flow rule.

1. Davoli, E. and Mora, M.G. 2012 A quasistatic evolution model for perfectly plastic plates, in preparation.

Determination of the equivalent anisotropy properties of polycrystalline magnetic materials: theoretical aspects and numerical analysis

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The aim of this talk is the determination of the equivalent anisotropy properties of polycrystalline magnetic materials, modeled as an assembly of monocrystalline grains with a stochastic spatial distribution of easy axes. The theory of Γ -convergence is here adopted to homogenize the anisotropic contribution in the energy functional and derive the equivalent anisotropy properties. The reliability of this approach is investigated focusing either on the micromagnetic computation of reversal processes and on the computation of the static hysteresis loops of polycrystalline magnetic thin films, starting from the numerical integration of the Landau-Lifshitz-Gilbert equation

1. O. Bottauscio, V. Chiadò Piat, M. Eleuteri, L. Lussardi, A. Manzin: *Homogenization of random anisotropy properties in polycrystalline magnetic materials*, Proceedings of the 8th International Symposium on Hysteresis and Micromagnetic Modeling, Physica B: Condensed Matter, **407**, no. 9 (2012), 1417-1419.
2. O. Bottauscio, V. Chiadò Piat, M. Eleuteri, L. Lussardi, A. Manzin: *Determination of the equivalent anisotropy properties of polycrystalline magnetic materials: theoretical aspects and numerical analysis*, submitted.

On a rate-independent modeling in damage

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We focus on the modeling of damage phenomena as rate-independent, activated processes. While the rate-independent theory seems to be well-established for systems with convex energy functionals, for non-convex energies there are interesting open problems, connected to the lack of regularity of the solutions as functions of time. The latter circumstance makes it necessary to recur to suitable weak solution notions. However, the by-now classical concept of global energetic solution fails to describe accurately the behavior of the system at jumps. In this talk, based on a joint collaboration with Dorothee Knees and Riccarda Rossi, we consider evolutions in damage driven by viscous, rate-dependent dissipation and discuss their vanishing-viscosity limit evolutions. By this procedure, we obtain a novel formulation for rate-independent problems, which highlights the interplay of viscous and rate-independent effects in the jump regime, and provides a better description of the energetic behavior of the system at jumps.

FOCUS SESSION

Mathematics & Industry, a novel approach to R&D

The exceptional growth of computational power of the last decade, together with a growing need for cost/effective product development process, allowed mathematics to gain importance in industrial applications.

With the development and diffusion of modelling and simulations techniques, favoured also by the launch on the market of easier to use multiphysics software tools, a new approach to mathematical support to R&D appeared. While, some years ago, mathematics was considered a part of the R&D process, mostly developed internally by company engineers, more and more, mathematics was seen as stand-alone part of projects. However, as the instruments needed to model and simulate complex processes with the required level of approximation grew in complexity, the support of highly specialized and skilled human resources became necessary. In order to satisfy this highly specialized market segment, it therefore resulted necessary to think of mathematics itself as the product of an industrial process.

The session focuses on this new approach to mathematics in R&D. The session concentrates on both aspects, *i.e.*, the growing need of highly specialized and refined mathematical modelling techniques, to support product/process development and quality control, and the skills made available by new market operators (enterprises or private R&D organizations) that “sell” mathematics for different applications in a new entrepreneurial approach.

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The oil industry: the kingdom of modelling

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Modeling flow in porous media: applications to solve industrial and environmental problems

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Industry informatics and mathematical intuition

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Modelling for industrial applications at MUSP laboratory

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Time seismic imaging without velocity model

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Applications of previsional mathematical models in the Smart Cities environment

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Mathematical methods for logistics hub operations and goods handling

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MOXOFF: mathematics for innovation

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LUNCH SESSION
**HPC at CINECA: overview, new features and applications in
mathematics**

The aim of CINECA's High Performance Computing Department is to develop and promote technical and scientific services for the Italian and European research community. It constantly invests in Supercomputing technologies, thus being able to provide researchers with some of the hardware resources among the most powerful in Europe. With this talk we would like to present to the Mathematics community what are the opportunities we can offer them and how can they use our resources for their computing simulations. Auditors will hear about the characteristics of the new HPC cluster "FERMI", that is going to be installed in a very short time. It will be also discussed how a potential user can have a totally free access to our resources for academic purposes, and how we interact with other European Supercomputing centres thanks to the PRACE project. A good part of the talk will be dedicated at showing some applications already benefitting of CINECA's clusters and covering various fields of Mathematics.

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