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Plenary Talks
Plenary Talks

New Trends in Complex Networks:
Temporal Networks

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Interacting agents moving over geographic space, functional relationships between the cortical areas of a brain during the performance of a task, messages and contacts over online social systems, are all examples of networks in which the links are frequently changing over time. All such systems have to be described in terms of temporal networks, i.e. time-ordered sequences of graphs defined over a fixed set of nodes. Concepts, metrics and models for static networks do not straightforwardly apply to temporal networks. In this talk we will discuss new metrics and models which allow to capture crucial information on the time ordering and possible concurrency of links in temporal complex networks from the real world. We will also investigate how the additional dimension of time influences collective processes.
From Individuals to Collectivity: Multiscale Methods for Living Complex Systems

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Dynamics of living complex systems, such as e.g., human crowds, cell aggregates, vehicular traffic, social systems, are mainly ruled by microscopic mutual interactions among the individuals, who continuously assess and revise their strategies of local movement. This originates self-organized collective trends, clearly visible by looking at the macroscopic group as a whole. A great challenge for mathematical modeling is to explain the spontaneous emergence of self-organized behaviors at large scale out of individual interactions at smaller scales. Various modeling approaches to the problem are currently studied in the literature, for instance: dynamical systems at the microscopic scale, macroscopic fluid dynamical models, (generalized) Boltzmann/Vlasov-type kinetic models, mean field games, cellular automata models. In addition, strategies to link models at different scales in a multiscale perspective are under intense investigation.

In this talk I will give an account of recent research on multiscale models for self-organizing living systems of the kind mentioned above, trying to relate the proposed mathematical methods to basic complexity features that such methods are supposed to catch. The contents of the talk are mostly taken from the works cited hereunder.


Variational models for dislocations

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In the understanding of plastic behaviour of metals a fundamental role is played by dislocations. These are line defects in the crystalline structure that favor the slip along slip planes, known to be the main mechanism for plastic deformation. These defects interact, move and organize in complex structures producing other important effects, such as hardening. Dislocations have been introduced theoretically at the beginning of the 20th century, in order to explain such effects, and then observed at the microscope many years later. In the last decades there have been considerable efforts to rigorously derive models for plasticity which could take into account effectively the presence and the interaction of such defects. The main goal is to describe the collective behaviour of systems of dislocations by means of a multi-scale analysis that starting from a microscopic, discrete, description containing all the relevant details of the crystalline structure, could give rise to a continuum model at the macroscopic scale. In its generality this task is very far from being completed, but many important steps have been made in special, but relevant, cases.

I will give an overview of some of the variational models for dislocations at different length scales and I will illustrate some recent results concerning the multi-scale analysis for dislocations via Gamma-convergence.
The construction of approximate methods of solution for the Boltzmann equation has a long history tracing back to D. Hilbert, S. Chapman and D. Enskog at the beginning of the last century but only in recent years, the problem has been tackled numerically with particular care to accuracy and computational cost. Even nowadays, however, the deterministic numerical solution of the Boltzmann equation represents a challenge for scientific computing.

Most of the difficulties are due to the multidimensional nature of the problem (usually a 7 dimensional problem, 6 space dimensions plus time) and to the structure of the collision integral which leads to the so-called curse of dimensionality. In addition the numerical integration requires great care since the collision term is at the basis of the macroscopic properties of the equation.

Therefore traditional grid-based methods are ineffective and the method of choice has been the Monte Carlo method. However, Monte Carlo method suffers from two difficulties. One is the slow convergence rate. The other is the numerical noise in the solutions. For this reason, it is still highly desirable to develop effective grid-based methods that solve directly the partial differential equations. In this talk we survey some recent progress in the development of efficient solvers based on spectral methods which permits to overcome the computational complexity of the Boltzmann equation.
Bibliography


Computational Concerns in Appearance Reproduction

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The introduction of 3D printing could change the dynamic of manufacturing forever by allowing everybody to print their own objects. This in turn changes the manner in which objects’ are designed, going from a specialty for technically savvy users to a mass movement. For this reasons, the Computer Graphics community as a whole is investigating new design paradigms to allow end-user to print novel objects with ease. My work focuses on using printers to reproduce the appearance of materials different than the ones used to print with. I will show that this is in fact possible with current hardware by solving carefully-constructed optimization problems.
Sampling and collocation methods for PDEs with random data

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In this talk we review sampling based techniques for the approximation of output quantities related to the solution of a partial differential equation with random input data. Such techniques evaluate the PDE and the corresponding output quantity only for specific (random or deterministic) values of the input data and therefore can use a PDE solver as a black-box.

We first consider global polynomial approximations of the input/output map and present sparse grid interpolation schemes on tensorized Gauss points that can handle a large number of input data. Some recent theoretical and numerical results will be presented for elliptic PDEs with random coefficients.

In the case of rough spatially distributed random data, polynomial approximations might become ineffective. We then turn to Monte Carlo approximations based on random sampling and their corresponding multilevel variants and show how coarse polynomial approximations can still be used effectively to accelerate the convergence of Multi-Level Monte Carlo estimators.


Minisymposia
Minisymposia

Data Assimilation: an ill posed inverse problem. Numerical topics and Applications

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Reliability of numerical methods is becoming a crucial issue as scientific computing has an increasing role in different fields of engineering and science (CSE: computational science and engineering). Models are far from perfect: due to the uncertainty in the initial conditions and computational limitations, models cannot provide accurate simulations. Observations measured by instruments provide direct information of the solution. Such observations are heterogeneous, inhomogeneous in space, irregular in time, and subject to differing accuracies.

Data Assimilation (DA) is the mathematical methodology for combining data acquired experimentally (in vivo, i.e. the reality or observational data) to those obtained numerically (in vitro, i.e. the background knowledge) in order to improve the understanding of complex systems or to improve the estimate of the system state (the forecast). To assimilate from the Latin just means to make similar.

In the past years DA, used in principle only in atmospheric models, has become a main component in the development and validation of mathematical models (often these models are referred to with the term predictive to underline that these are dynamical systems). The issue of assimilating data into models arises in all scientific areas that enjoy a fusion of data.

The DA is an inverse and ill posed problem: retrieve the system state from sparse and noisy observations. Historically, the communities of inverse problems and data assimilation have evolved independently, with particular notation and approaches which are similar in content, but have been expressed in different type of notation or terminology. Understanding important state-of-the-art algorithms within a uniform framework is a key step today to further develop the computation tools which are known to have the highest impact on society, breaking down barriers to research and innovation (Horizon 2020). The Workshop on Data Assimilation addresses key concepts arising from both numerical algorithmic developments (regularization, preconditioning, efficiency, scalability,) as well as from important applications (in oceanography, medical imaging, geosciences, ..).
Many important image processing applications in medicine and astronomy, such as the deblurring of astronomical or medical images acquired through optical devices (telescopes, microscopes) and the noninvasive acquisition of relevant biochemical information from magnetic resonance spectroscopy imaging, are extremely relevant problems in the scientific area with a meaningful social effect. The development of efficient methods and algorithms for their solution is an actual research topic because the algorithms implemented on the commercial systems are often too slow or too sensible to noise on the data. Moreover, they do not determine numerical solutions preserving specific image properties such as, for example, the edges of the bone tissue images or the bright of star cluster images.

The aim of this symposium is to collect several experiences of real applications in image processing addressed by means of effective numerical linear algebra and optimization approaches. Since several difficulties in imaging problems are related to the corruptive effect of the noise affecting the data, the symposium is open to recent general results on inverse problems and regularization approaches.

Particular attention will be devoted to the description of the numerical complexity which characterizes the particular applications and the applicability to large-scale problems, possibly with the support of parallel architectures. Contributions to Krylov or Arnoldi-Tikhonov methods, first and second order optimization methods, dual or primal-dual approaches and non-negative factorizations will be considered.
New developments and applications of Groebner bases

Gröbner bases are a universal tool for any kind of problems that can be modeled by polynomial equations and one of the most powerful methods in commutative algebra and algebraic geometry, but the range of theoretical issues and applications related to Gröbner bases is enormous. It includes theoretical physics, applied science and engineering since many problems in mathematics, applied science and engineering can be represented by polynomials (ideals, modules, matrices, ...). Gröbner bases have been used by researchers in optimization, statistics, coding, signal and image processing, computer vision science and in the field of security, to encrypt messages or to transmit confidential information. The Gröbner bases technique has been implemented in mathematical software systems like Mathematica, Maple, CoCoA, Macaulay. Classes of ideals in polynomial rings can be investigated via Gröbner bases in order to introduce algebraic objects useful in some applications and to provide efficient algorithms. The study of the data obtained from the implementation and their processing can be a useful support for the development of the research. The goal is to show how algebraic and geometric models built through Gröbner bases theory are useful for setting suitable solutions of several real problems concerning different areas. The proposal covers recent developments within this context, in order to translate or evaluate theoretic results into concrete examples.

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Complex Systems (SisCo-SIMAI Activity Group)

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This is the minisymposium of the SIMAI Activity Group on Complex Systems (SisCo-SIMAI), which gathers scholars interested in the study of complex systems through methods of mathematical modeling. The group promotes the development of modeling methods soundly based on mathematical structures able to deal with the typical features of complex systems: nonlinear interactions among the constituents, spontaneous emergence of collective behaviors and self-organization, multiscale issues, stochasticity, and many others.

In this spirit, the minisymposium proposes a few contributions, mostly from the members of the Activity Group, which cover a quite wide spectrum of applications in the field of complex systems: vehicular traffic on road networks and related safety issues, crowd dynamics with control and optimization of evacuation strategies, cooperation vs. competition and selection dynamics in biological and social systems. Attention is paid also to foundational aspects, particularly the study of suitable theories which can serve as general frameworks for addressing complex systems from a rigorous mathematical point of view.

All of the applications mentioned above have a great social and industrial impact on modern societies, for instance as far as the design of the so-called “smart cities” is concerned. They are therefore expected to be relevant for the scope of SIMAI.
Mathematical Models and Computational Methods in Biomedicine

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This symposium aims at illustrating four problems in which the availability of an accurate mathematical model and the application of a sophisticated computational method allow the comprehension of crucial and to many extents open physiological and biological issues. Three of such problems have immediate or prospective clinical applications and are concerned with, respectively: the determination of a novel prognostic parameter for the assessment of chronic leukemia; the description of cancer metabolism in a comorbidity context, using nuclear medicine data; the identification of dynamical patterns evoked in the brain by somato-sensory stimulation. The fourth problem involves the determination of the size of proteins (and, in general, nano-structures) by using small angle X-ray scattering. From a mathematical perspective, the workshop will offer the description of a wide set of up-to-date computational methods, ranging from statistical inversion algorithms all through inverse scattering methods, Sequential Monte Carlo samplers, Bayesian filters, pattern recognition approaches and computational geometry arguments. Finally, all four talks will present analysis of experimental data (some of them collected in clinical contexts) and discuss the results in frameworks provided by interdisciplinary collaborations involving oncologists, radiologists, neuroscientists, bioengineers and nanoscientists.

Talk 1 (biological structures)

Title
A Small Angle X-ray Scattering Technique for Determining Nano-scale Particle Size Distributions

Speaker
Federico Benvenuto, Centre de Mathematiques Appliquees, Ecole Polytech-
Abstract
The determination of a protein's scale size is a difficult problem that is typically addressed by means of crystallography. Small angle X-ray scattering (SAXS) may offer an alternative approach, which does not require the availability of a crystalline sample. Further, SAXS allows dynamic measurements and provides access to information not limited to the surface of the sample, being able to measure inside the material without sophisticated sample preparation. A SAXS experiment typically produces a one-dimensional scattering intensity obtained by circular averaging the 2D scattering pattern observed in the experiment. In order to determine the size information from this intensity, one needs to solve an ill-posed inverse scattering problem. This talk briefly introduces the SAXS modeling under the assumption that all nanoparticles in the system of interest are equally sized and shaped, and presents a statistical method to determine the size of the nanoparticles. SAXS data are obtained by an azimuthal re-groupment of scattered photons acquired by a charged coupled device and therefore are Poisson distributed. The talk will show the effectiveness of Expectation Maximization, when coupled with an appropriate stopping rule, to retrieve positive parameters from SAXS data.

Talk 2 (neural sources)

Title
Sequential Monte Carlo Samplers for the determination of neural activity from neurophysiological data

Speaker
Alberto Sorrentino, Dipartimento di Matematica, Università di Genova

Abstract
Magnetoencephalography (MEG) records non-invasively the magnetic fields produced by the brain. In the dipolar approximation, the neural current is modeled as an unknown number of point sources, termed current dipoles. We consider the problem of estimating the number of dipoles, their location and strength, from a single spatial distribution of magnetic field. We use a Bayesian approach, with uninformative priors for all parameters but the number of sources, which is assigned a Poisson prior with low mean. We set up a sequential Monte Carlo sampler that samples from a tempering se-
quence (a one-parameter family) of distributions, which closely reminds the regularization path. From the so-obtained posterior distribution we compute point estimates of the source parameters. Simulated data show very good localization properties, and experimental data evoked by somato-sensory stimulation confirm that the method can localize sources in real scenarios.

**Talk 3 (systems physiology)**

**Title**
Compartmental Models for Nuclear Medicine Data: an Inverse Problems Perspective

**Speaker**
Michele Piana, Dipartimento di Matematica, Università di Genova

**Abstract**
Compartmental analysis is a computational tool for the modeling of nuclear medicine data that, in its most recent applications, exploits spatio-temporal information provided by Positron Emission Tomography (PET). This talk introduces two novel compartmental models describing the processing of 18Fluorodeoxyglucose (FDG) in the renal and hepatic systems. The first model accounts for variations in FDG concentration due to water re-absorption in renal tubules and for increase of bladder’s volume during the excretion process. The second model accounts for the dual blood supply proper of the liver circulatory system and uses tracer concentration in the gut to describe the flow in the portal vein at the liver entrance. The computational reduction of both models is performed by using inverse problems techniques: in the first case we used a non-stationary steepest descent approach that explicitly accounts for the Poisson nature of nuclear medicine data; in the second case, we applied a regularized multi-dimensional Newton algorithm with an ad hoc rule for the optimal selection of the regularization parameter. The applications considered illustrate new insights about the role of metformin in cancer metabolism and utilizes data recorded by a PET system for small animal models.

**Talk 4 (clinical application)**

**Title**
The Hough Transform and a Novel Prognostic Index for Chronic Leukemia
Abstract
It has been recently proved that a computational analysis of Positron Emission Tomography / Computerized Tomography (PET/CT) images allows the assessment of alteration of bone structure and bone marrow metabolism in adult patients with advanced chronic lymphocytic leukemia and that this kind of analysis may even offer prognostic potentials. The crucial requirement for the reliability of this study is the application of a pattern recognition method able to accurately segment the intrabone space in clinical CT images of the human skeleton. The talk shows how this task can be accomplished by a procedure based on the definition of Hough transform for special classes of algebraic curves. The idea is the one to introduce a catalogue of curves that satisfy some specific algebraic geometry conditions, to compute their Hough transform and apply a standard recognition approach based on the optimization of an accumulator function. The effectiveness of this method will be proved against low-resolution clinical CT data and lead to the recognition of complex profiles in many different districts of the human skeleton.
New perspectives on applicabilities in graph theory

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Abstract/Short description
Graph theory is becoming increasingly significant as it is directed to other areas of mathematics, science and technology. It is being actively considered in fields as varied as biochemistry, physics, statistics, engineering, computer science, and so on. More in detail, graphs can be used to model many types of relations and processes in scientific systems: all transport networks can be sketched by graphs in one way or the other; a telecommunication system (mobile telephone networks or internet) can also be described as a network; coding theory is actively developed by planning configurations of graphs; servers can be reproduced as nodes within a graph while the physical infrastructure between them, namely fiber optic cables, can act as links; even for assembly lines in the industry one can refer to graphs; not least, in computer science, graphs are introduced to represent networks of communication, data organization, optimization problems, the flow of computation, research algorithms for the web. Graph theory is also considered for studying molecules in chemistry, genomics and statistical physics: in chemistry, a graph makes a natural model for a molecule, where vertices represent atoms and edges bonds, and this approach is especially used in computer processing of molecular structures, ranging from chemical editors to database searching; in genomics, significant structures that give a real description of DNA sequencing methods may be illustrated by means of graphs; in statistical physics, graphs can represent local connections between interacting parts of a system, as well as the dynamics of a physical process on such system. The powerful combinatorial methods found in graph theory have also been employed to prove fundamental results in other fields of pure mathematics. Classes of graphs can be studied using computational and algebraic procedures in order to introduce patterns in several practical problems. More
precisely, algebraic objects associated to a graph are special classes of monomial ideals such as edge ideals, vertex covers ideals, paths ideals. Monomial ideals are one of the keys intersections between commutative algebra and combinatorics. In particular, in the square-free case, their connection with algebraic graph theory and simplicial complexes is a crucial point for the applications in different fields of commutative algebra and algebraic geometry.

Motivation/Relevance to SIMAI
The present minisymposium explains how commutative algebra, linear algebra, graph theory and combinatorics could help applied science and give solutions for real problems concerning different technological areas. The aim of it is to inform about some recent surprising developments supported by graphs, to show nice applications in the vast field of action for graph theory, to bring together experts which constitute different branches of research and to stimulate the exchange of ideas.

Confirmed/Proposed speakers

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Numerical methods for coupled problems

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Modeling many physical phenomena requires to study problems of multi-physics and/or multi-scale nature. For example, this is the case in highly structured flows in fluid dynamics, in structural mechanics, in viscous-inviscid fluid interactions, in heterogeneous materials, in electromagnetism or in geophysical and biomedical applications. The complexity of the underlying processes often poses a challenge at both the analytical and the numerical level. In particular, special care has to be paid at the choice of the coupling conditions between the different models and to their mathematical treatment in order to ensure the well-posedness of the global system of equations. Moreover, effective and reliable algorithms involving robust preconditioning techniques must be considered. These numerical schemes can be based on either segregated or monolithic methods. In this minisymposium we would like to bring together experts in coupled problems to discuss the model derivation, their theoretical mathematical properties, as well as the set-up and analysis of efficient numerical tools.

Motivation/Relevance to SIMAI
We believe that the discussion of the numerical solution of various coupled problems should be of interest for SIMAI since many practical and industrial problems rely on the coupling among different phenomena.

Confirmed speakers

1. Paola Gervasio, Dipartimento di Ingegneria Civile, Architettura, Territorio, Ambiente e di Matematica, Università di Brescia
2. Ana Alonso, Dipartimento di Matematica, Università degli Studi di Trento
3. Lucia Gastaldi, Dipartimento di Ingegneria Civile, Architettura, Territorio, Ambiente e di Matematica, Università di Brescia
4. Edie Miglio, MOX, Dipartimento di Matematica, Politecnico di Milano
5. Annalisa Quaini, Department of Mathematics, University of Houston
6. Nicola Bellomo, Department of Mathematical Sciences, Politecnico di Torino
7. Simone Palamara, MOX, Dipartimento di Matematica, Politecnico di Milano
8. Alessandro Colombo, Dipartimento di Ingegneria, Università di Bergamo
9. Fabrizio Del Bianco, Dipartimento di Ingegneria Industriale e dell’Informazione, Università di Pavia
10. Luca Gerardo-Giorda, Basque Center for Applied Mathematics
11. O. Rheinbach, Technische Universität Bergakademie Freiberg, Fakultät für Mathematik und Informatik

Other proposed speakers
Nicola Parolini, MOX, Dipartimento di Matematica, Politecnico di Milano
Minisymposia

Computational models for natural hazards and extreme events simulation

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Natural disasters, such as atmospheric, hydrologic, oceanographic, volcanologic and seismic events, have a catastrophic impact on the modern society in terms of human, economic and environmental loss. For enhancing the mitigation of hazards and decreasing the risk, advanced computational techniques are recognized to represent an effective tool for data analysis, early warning and planning purposes. In this minisymposium we aim to discuss recent developments on all aspects of natural hazards and extreme events simulation, from the forecasting of catastrophic events to the risk management. Particular attention will be devoted to recent advances on numerical methods for the simulations of extreme events, challenging in code development and implementation of the models on modern supercomputers.

Tentative List of Speakers

1. Marino Marrocu, CRS4 (to be confirmed)
2. Ilario Mazzieri, MOX, Politecnico di Milano (confirmed)
3. Giovanni Russo, Universit di Catania (confirmed)
4. Augusto Neri, INGV Pisa (confirmed)
5. Giovanni Tumolo, ICTP, Trieste (confirmed)
6. Marco Stupazzini, MunichRe (to be confirmed)
Variational Inequalities, Immune Systems and Local Minimizers of Functionals

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Main goals of Minisymposium are Variational Inequalities, Immune Systems and Partial Regularity of Local Minimizers. The first one is considered in the context of equilibrium problems and network design, the second and third arguments are treated in a more theoretical sense.

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, traffic network equilibrium problems, vaccination problem, oligopolistic market equilibrium problem and financial problem. In particular, when considering the above problems in their evolution in time they are modeled by evolutionary variational inequalities. Several classical and new theories, such as those of 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.

Other argument concerned with analytical investigations on the competition between cancer cells and immune system cells. The mathematical models is a Kolmogorov-type systems of three evolution equations where the growth rate of the cells is described by logistic law and the response of cancer cells and immune cells is modeled according to Holling type-II function. The stability analysis of equilibrium points is performed and the persistence of the model is proved.
Moreover, the Minisymposium treated everywhere Hölder regularity in the interior for a minimizer of the $p(x)$ energy functional.

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.
Modeling, simulation and optimization of complex systems using Partial Differential Equations

The aim of this mini-symposium is the presentation of recent results on model, simulation and optimization studies based on Partial Differential Equations with applications to flows on vascular networks, flow of an incompressible, quantum behavior of a particle in an electric field, supply chains and traffic train. In particular, the modeling and the analysis of wave propagation phenomena along spatial networks (such as vascular networks), inspired from (and with applications to) modeling blood flow in the cardiovascular network is considered. For a spatial network such as the vascular network, the dynamics is typically described first at the level of individual edges, then at junctions, then at parts of the network, and finally, if feasible, at the level of the entire system. The aim is to study the effect of truncation to the flow in the root edge in the case of a self-similar tree or network, the effect of adding or subtracting an edge to a given network. The study of pulse propagation can help understand the pulse waveforms measured in-vivo and the effects of anastomoses in some arterial networks. As regards the model of a particle in an electric field, it is given by the Schrödinger equation. Of relevant importance is the ground state of the particle and it can be related to the heat kernel of the differential operator. For this reason, it can be useful to study the kernel of the semigroup generated by a Schroedinger type operator with unbounded coefficients. About the supply chain, the problem to adjust the inflow to a supply chain in order to achieve a desired outflow, reducing the costs of inventory or the goods timing in warehouses is studied. The supply chain is modeled by a conservation law for the density of processed parts coupled to an ODE for the queue buffer occupancy. The control problem is stated as the minimization of a cost functional measuring the queue size and the quadratic difference between the outflow and the expected one. The controls are the discontinuity points of the input flow chosen as a piecewise constant function. The same techniques can be applied in some optimization problems. For instance, in collaboration with Trenitalia and Bertolotti, it was considered a model to optimize the train traffic between Germany and Italy.

Speakers

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GASVA minisymposium on Mathematical Modelling in Environmental and Life Sciences

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The minisymposium aims at presenting the scientific results achieved by the members of the SIMAI activity group on Environmental and Life Sciences. Several mathematical models will be described with application to cancer modelling, chemotherapy, morphogenesis, cell motion, tissue remodelling and regeneration, protein networks, systems medicine, genetics, stem cell behaviour, biofilms, and environmental remediation strategies. Eight researchers have already confirmed their participation. Others may join. It might be foreseen that the participant will fill three mini-symposia, one more specifically oriented to environmental applications and the other two on bio-medical applications, possibly more biologically oriented and one more medically oriented. For this reason more specific abstracts will be available when the final list of speakers will be known.
We propose to organize a minisimposium within the Simai meeting on the topic “Numerical methods and models for multiscale kinetic equations”

Kinetic equations are a tool to model phenomena on a macroscopic scale which are influenced by the behavior of the microscopic particles composing the system. These models are particularly effective on multiscale problems when part of the system may have reached equilibrium (and thus the microscopic scale can be underresolved) while in other regions the system can be far off equilibrium and here the microscopic scale must be resolved even if one is interested only in the macroscopic effects.

These models arised initially in gas dynamics, and have since been applied to many other fields in physics, applied sciences, and even biological and social sciences. The potential for applications in so many fields makes these models particularly suited for SIMAI, because their success in applied mathematics and physical modeling is well established, while their exploitation in industrial applications is still in its infancy.

This minisimposium is designed to gather recent contributions to the field. In particular, we will concentrate on the modeling of mixtures of different populations of particles, which can exchange momentum and energy (as in plasmas) or even mass (as in chemical reactions). Moreover, the minisimposium will address also researchers interested in the numerical treatment of these equations, with particular emphasis on Asymptotic Preserving schemes, which are designed to bridge the gap between microscopic and macroscopic scales, with no need to resolve the fast scales of transient phenomena.
Speakers who have already agreed to deliver a talk at the minisimposium are:

Giacomo Albi (University of Ferrara, PhD student): Flocking, Consensus formation, AP schemes and control

Gian Pietro Ghiroldi (Politecnico of Milano) Relaxation of vibrational-rotational modes in polytropic gases

Maria Groppi (University of Parma, Associate Professor) Modeling of kinetic mixtures, chemical reactions

Christian Klingenberg (University of Wuerzburg) Plasma modeling and numerics for MHD equations

Giuseppe Stracquadanio (University of Parma) Lagrangian AP schemes for the BGK equation

Potential speakers who will receive an invitation if the minisimposium is accepted are:

Stephane Brull (University of Bordeaux)

Nicolas Crouseilles (Inria Rennes)

Luc Mieussens (University of Bordeaux)

Vittorio Rispoli (University of Toulouse)

Giovanni Russo (University of Catania)
Proposal of minisymposium: The mathematics of learning from data

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The last few years have seen an unprecedented growth in the scale, structure and complexity of data in science and engineering. Machine learning has become key to analyze these data, and nowadays enables systems such as Siri, Kinect or Google self driving car, to name a few examples. At the same time machine learning methods help deciphering the information in our DNA and make sense of the flood of information gathered on the web. It is widely recognized that a main reason for this success has been the development of a solid mathematical foundation of machine learning algorithms. Learning theory is nowadays becoming a mature field in the mainstream of mathematics. The goal of this mini-symposium is to gather experts to provide an overview of the state of the art and challenges in the field, and highlight the connections of Learning Theory with other fields such as optimization, high dimensional probability and inverse problems among others.
Particle laden turbulent shear layers have recently received a very much increased attention due to the possibility to simulate those flows accurately at high Reynolds numbers. This mini-symposium concentrates on shear layers for example jets and boundary layers. Contributions from highly resolved numerical simulation in the compressible and incompressible flow regime are solicited. Applications for for industrial and geophysical applications like volcanic jets or pyroclastic density currents are welcome.

confirmed papers:
- Riccardo Scatamacchia, Federico Toschi and Luca Biferale
- Carlo Massimo Casciola
- Matteo Cerminara, Tomaso Ongaro Esposti
- Arne Heinrich, Flavia Cavalcanti, Jörn Sesterhenn

possible speakers:
- Markus Uhlmann
- Paolo Gualtieri
Discrete and continuous models for pedestrian movements

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The mathematical modelling of the motion of pedestrians is increasingly attracting the interest of applied mathematicians. This is both due to the interest in the applications (see next section “Motivation”), and due to the challenging mathematical structure of the model arising.

Several models for the movement of crowds have been proposed in the literature. One can distinguish between two general approaches: microscopic and macroscopic models. In the microscopic framework, people are treated as individual entities (particles). The evolution of the particles in time is determined by physical and social laws which describe the interaction among the particles as well as their interactions with the physical surrounding. Examples for microscopic methods are social-force models (cf. Helbing 2002 and the references therein), cellular automata, e.g Fukui 1999 and Muramatsu 2000.

In contrast to microscopic models, macroscopic models treat the whole crowd as an entity without considering the movement of single individuals. Classical approaches use well known concepts from fluid and gas dynamics, see Henderson 1971. More recent models are based on optimal transportation methods, cf. Santambrogio 2009, mean field games (see Burger-DiFrancesco-Markowich-Wolfram 2013) or non-linear conservation laws, cf. Colombo2005. In Piccoli2009, an approach based on time-evolving measures is presented. In 2012, Burger-Markowich-Pietschmann-Wolfram proposed a cellular automata approach leading to a continuum limit resembling a chemotaxis model. Starting from the paper by DiFrancesco-Markowich-Pietschmann-Wolfram in 2011, a great attention has been given to the so called Hughes model, a conservation law based model with a non local discontinuity which makes the existence theory a hard task, see Amadori-Di Francesco 2012 and Amadori-Goatin-Rosini 2013.
The proposed mini symposium will review the latest advances in this field, in both the theoretical analytical context and the numerical one. Contributions will focus in particular on nonlinear transport type models, possibly with constraints, with possible connections to control problems. The interplay between microscopic ODE based models and macroscopic mean field equations will be also addressed. Particular attention will be devoted to the Hughes model, with the leading experts in the field among the proposed speakers (Debora Amadori and Massimiliano Rosini). Monika Twarogowska will report of her numerical work with Paola Goatin et al. on a similar class of models. Marco Di Francesco will present a review on transport models for the movement of pedestrians. If the participation of Marie Therese Wolfram is confirmed, she will present recently developed models based on the mean field games theory, with several collaborators (M. Burger among others). Carlotta Donadello (if confirmed) will present a recent paper on a transport model for pedestrians with constraints. Fabio Priuli will present a result in collaboration with Tosin and Cristiani on controlling self-organization of pedestrians by modelling the rationality of the individuals.

We would be delighted to have the participation of Nicola Bellomo, who is a world leading expert on the field. Jon Dawes (Bath) is another possibility (he is currently checking possible clashes with other events, he developed simulations on a simple ODE based model trying to detect Maurys turning condition). We are also considering the possibility of inviting Boris Andreianov as a back-up plan. NOTE: the organizer would cancel his own name from the list of speakers if the total number of speakers gets strictly larger than 8.

**Motivation/Relevance to SIMAI:**
The mathematical modelling of large human crowds has gained a lot of scientific interest in the last decades. This is due to various reasons. First of all, a very serious issue in this context is to shed a light on the dynamics in critical circumstances. Moreover, the analytical and numerical study of the qualitative behaviour of human individuals in a crowd with high densities can improve traditional socio-biological investigation methods. The dynamics of a human crowd has also applications in structural engineering and architecture: the London Millennium Footbridge which had to be closed on the day of its opening due to unexpected anomalous synchronization, is a very evocative example in this sense. Other applications of pedestrian flow modelling arise in transport systems, spectator occasions, political demonstrations, panic situations such as earthquakes and fire escapes. More light-
hearted examples are the simulation of pedestrian movement in computer games and animated movies. Another important application is related with the development of smart building / smart cities, in which the descriptive power of mathematical models for the motion of pedestrians can be of great help in optimal architectural design and urban planning.

Confirmed speakers:

1. Debora Amadori (University of LAquila)
2. Marco Di Francesco (University of Bath & University of LAquila)
3. Fabio Priuli (IAC-CNR Rome)
4. Massimiliano Rosini (University of Warsaw)
5. Monika Twarogowska (IAC-CNR Rome)

Other proposed speakers:
Speakers who have been contacted and for whom I am awaiting for a confirmation:

1. Marie-Therese Wolfram (University of Vienna)
2. Carlotta Donadello (Universitè de Franche-Comtè, Besanon)

Other possible speakers:

1. Nicola Bellomo (Politecnico di Torino)
2. Jonathan Dawes (University of Bath)
3. Boris Andreianov (Universitè de Franche-Comtè, Besanon)
“Mathematical Applications funded by the European Union”

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The European Union provides funding and grants for a broad range of projects and programs, managed by different bodies. If the funds are managed by one of the member countries, they are known as structural funds and usually finance regional policy, social and training programs, as well as agriculture (including support for farmers). There exist two kinds of funding: the first one are grants for specific projects, usually following a public announcement known as a “call for proposals”, while the second one are public contracts, in order to buy services, goods or works and to ensure the operations of the EU institutions or programs. Contracts are awarded through calls for tenders (public procurement) and involve a wide range of areas: research, training and technical assistance, expert advices, conference organization, Information Technologies equipment purchases, and so on. The EU has approved an Operational Program for Sicily (PO) with the aim of promoting the development of the region through aids to business and intervention strategy for tourism sector, basic infrastructure and environmental protection. Common funding comes from the European Regional Development Fund (FESR), the European Social Fund (FSE) and the European Agricultural Guidance and Guarantee Fund (FEAOG). The main actions planned for the FESR involve industry, crafts and business services (such as support for business start-ups, improving the facilities in industrial and craft areas, etc.), tourism (i.e. better accommodation, notably rural, touristic infrastructure, preservation of the cultural heritage), infrastructure to support economic activity (relating to water distribution and supply, energy sources, scientific research and development, technological innovation,
research facilities at universities and urban rail transport), the environment
(as improving waste-water treatment capacity, treatment of solid waste from
urban centers and hospitals, measures to prevent coastal erosion and im-
provement of protected natural areas), and technical assistance. Within the
PO FESR 2007-2013, support action to industrial research and experimen-
tal development activities have been activated in connection with supply
chains, technological districts and production in potential excellence areas
that test a high degree of integration between universities, research centers,
SMEs and large enterprises. Some projects funded by this grant have been
developed and conducted by using mathematical modeling and application
to specific problems. Because of the multidisciplinary of the topic treated, it
is crucial a joint work between mathematicians, computer scientists and en-
gineers and it is noticeable the need for mathematical and numerical models.
Some of these projects will be presented in this Mini-symposium, emphasizing
their industrial and technological application.

Motivation/Relevance to SIMAI:
This Mini-symposium proposes to point out practical and concrete applica-
tions of the mathematics from problems emerging from the SMEs needs and
to underline the close relationship and connection between scientific research
developed at the universities and the world of work and industry.

Confirmed speakers:

Dott. Giorgio Grasso (University of Messina);

Ing. Mauro De Marchis (University of Enna Kore);

Ing. Andrea Alaimo (University of Enna);

Ing. Luca Trefiletti (University of Enna Kore)

Other proposed speakers:

Ing. Giovanni Garaffo (Demetra S.r.l).
Models and applications of the theory of conservation laws

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The aim of the minisymposium is to give an up to date account of different aspects of conservation laws and their applications.

Speakers:

- Sara Daneri, Leipzig University
- Marco Di Francesco, Bath University
- Marco Sammartino, Università di Palermo
- Laura Spinolo, CNR Pavia
The goal of the mini-symposium is to provide a forum which brings together researchers who study various aspects of nonlinear waves and pattern formation using analytical and numerical techniques among different fields of application. The mini-symposium program will consist of presentations on subjects ranging from basic mathematical research (existence and stability issues), to concrete applications.

Motivation/Relevance to SIMAI:
Theoretical aspects of applied mathematical research on nonlinear waves and coherent structures are relevant to subjects as fluid and solid mechanics, atmosphere and ocean dynamics, chemical reactions and biology, heat transfer and thermodiffusion effects of mixtures, high-energy particle and plasma physics. Remarkable agreement between theory and experiments can be claimed in many of these fields.

Confirmed speakers:

1. Francesca Brini, Dipartimento di Matematica, Università di Bologna, francesca.brini@unibo.it;
2. Giuseppe Maria Coclite, Dipartimento di Matematica, Università di Bari, coclite@gm.dm.uniba.it;
3. Deborah Lacitignola, Dipartimento di Ingegneria Elettrica e dellInformazione, Università di Cassino e del Lazio Meridionale, d.lacitignola@unicas.it;
4. Francesco Paparella, Dipartimento di matematica, Università di Lecce, francesco.paparella@unile.it.

Other proposed speakers:

1. Andrea Giacobbe, Dipartimento di Matematica, Università di Padova, giacobbe@math.unipd.it;

2. Giovanni De Matteis, Dipartimento di Matematica, Università di Milano, giovanni.dematteis@unimi.it.
Minisymposia

Signal and image processing techniques, and applications

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The proposed mini-symposium is related to the activities of the SIMAI Activity Group “SIMAI-SIMA”, whose aim is to promote and coordinate research activities on mathematical models and numerical methods for experimental data analysis, CAGD, automation, animation, signal processing, image processing, scientific visualization, virtual reality. The mini-symposium is intended to bring together researchers from different fields working on signal and image processing with the aim of presenting and sharing novel techniques, research results, and experience. A special emphasis will be put on the applications to real-world problems, principally including biomedical applications. In particular, the talks included in the mini-symposium will present research advances both in the aspects related to the construction of suitable methods for data analysis (fuzzy techniques, image fault detection, radial basis functions, multiple MRA) and in the application of data processing techniques to real problems (EEG, Electroanatomy, MEG, Functional Near Infrared Spectroscopy, magnetic tomography)
From computer aided geometric design to industrial CAD modeling and simulations

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Short description  Computer aided geometric design (CAGD) methods are devoted to the mathematical foundations of modern modeling and processing applications connected to scientific visualization and manipulation of geometric entities. CAGD–oriented algorithms deal with the effective construction, representation and manipulation of curves, surfaces, volumes and (computational) grids. The resulting geometric model has a key role for the subsequent elaboration in different industrial applications, including manufacturing and engineering simulations.

Even if commercial CAD (Computer Aided Design) systems rely on robust and accurate software libraries, the availability of highlevel technologies open the path to innovative solutions able to face challenging requirements emerging in industrial applications. Among others, representations of curves and surfaces possessing suitable algebraic/geometric properties or spline models not confined to the tensor–product polynomial structure are key ingredients for powerful and brand–new technologies. Related developments and their suitable interface with industrial geometric modeling standards seems to be the challenge that the research and CAD community has to face.

The minisymposium will focus on emerging scientific results in the field, as well as on relevant applications of established techniques in the industrial environment.
Motivation/relevance to SIMAI  CAGD methods have a key role in different industrial applications, including manufacturing and engineering simulations and represent a relevant up-to-date topic in applied mathematics. They constitute a natural bridge between academic research and the technological environment in industry.
Several systems of evolutionary partial differential equations may contain stiff terms, which require an implicit treatment. Typical examples are hyperbolic systems with stiff hyperbolic or parabolic relaxation and kinetic equations in regimes close to fluid dynamic limit. In many cases, the stiff terms are clearly identified. For example, in hyperbolic systems with hyperbolic relaxation, the hyperbolic term is usually non stiff, while the relaxation term is stiff. A natural way to treat such systems is to adopt implicit-explicit schemes, in which the relaxation is treated by an implicit scheme, while the hyperbolic part is treated explicitly. In several cases, however, such a distinction is not so clear. For example, in the case of hyperbolic systems with diffusive relaxation, a standard approach would lead to schemes, which in the stiff limit suffer from classical parabolic CFL restriction. Such systems can be treated by a penalization method, consisting in adding and subtracting the same term, so that the system appears as the limit relaxed system plus a small perturbation. There are cases, however, in which stiff terms are not just additive, and the penalization method is not particularly effective, since the limit system itself is not easily solvable by standard techniques. For many such systems, we present a new approach, which includes partitioned and additive approach. It consists in identifying the linearly stiff dependence of the system on the unknown variable. Only this linear dependence will be treated implicitly, while the rest of the system is treated explicitly. This approach generalizes classical IMEX schemes based on additive or partitioned Runge-Kutta methods, and allows the construction of high order linearly implicit schemes, which are much simpler to use than fully implicit ones. Several examples will be presented.
Mathematical Problems from micro ans nano-electronics industry

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Organizers: Giuseppe Ali, Giovanni Mascali, Orazio Muscato, Vittorio Romano

Modern electron devices require an increasingly accurate modeling of energy transport in semiconductors in order to describe high-field phenomena such as hot electron propagation, impact ionization and heat generation. The standard drift-diffusion models cannot cope with high-field phenomena since they do not comprise energy as a dynamical variable.

Also for many applications in optoelectronics it is necessary to describe the transient interaction of electromagnetic radiation with carriers in complex semiconductor materials and since the characteristic times are of order of the electron momentum or energy flux relaxation times, some higher moments of the carrier distribution function must be necessarily involved. These are the main reasons why more general models have been sought which incorporate at least energy as a dynamical variable. In recent years new studies have been carried out whose main scientific achievements have been:

1. the development of physics based extended hydrodynamical models for submicron devices which do not have any free phenomenological parameters;

2. the numerical implementation of the transient extended hydrodynamical models based on the exploitation of higher order conservative schemes for hyperbolic systems of conservation laws;

3. the numerical implementation of the stationary extended hydrodynamical models by utilizing mixed finite elements;

4. the development of a deterministic (not Monte Carlo) solver of the semiclassical Boltzmann transport equation for submicron devices;

5. the improved efficiency of Monte Carlo simulations.
The use of new materials, and the transition from microtechnology to nanotechnology undermine the reliability of the models classically used for the simulation of semiconductors. This fact requires the development of innovative research in advanced mathematics.

The objective of this minisymposium is to present the latest developments, insights, methods and ideas in the above areas of research, and indications for future research directions. An important aspect will be the involvement of researchers working for industries, which can provide a more timely indication of the most relevant up-to-date problems and technique encountered in real industrial environments.

_Tentative list of speakers:_

- Giuseppe Ali
- Roberto Beneduci
- Vito Dario Camiola
- Vincenza Di Stefano
- Concetta Drago
- Giovanni Mascali
- Orazio Muscato
- Vittorio Romano
Recent advances on the theory and applications of Semi-Lagrangian methods

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Large time-step or Semi-Lagrangian (SL) techniques have received a remarkable attention from the numerical PDE community in the last decade. In addition to the usual fields of application of such techniques, literature reports successful application of schemes of this class to new models, especially in nonlinear/nonsmooth situations modeled by first and second order Hamilton-Jacobi equations. At the same time, a more complete theoretical analysis and a deeper understanding of the features of this approximation strategy have been achieved. The minisymposium tries to give an update of recent developments, on the side of both theory and applications, of SL schemes. Special focus will be given to second-order equations, flux-form and high-order schemes.

Motivation/Relevance to SIMAI:
Current developments of SL schemes enlarge their range of use to new problems and models, of great interest for applications. In particular, perspective speakers of this minisymposium work on a variety of topics like atmospheric CFD, dynamic programming, flow in porous media, image processing, kinetic and multi-agent systems.

Speakers (confirmed):
- Luca Bonaventura (MOX Milano)
- Elisabetta Carlini (“Sapienza” Roma)
- Silvia Tozza ("Sapienza" Roma)
- Giovanni Tumolo (ICTP Trieste)

Other possible speakers (to be included if possible):
- Giuseppe Straquadanio (Parma)
- Emiliano Cristiani (IAC-CNR)
Contributed Talk
Development of a family of cost-optimized prefactored high-order compact schemes for low-speed aeroacoustics

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A new class of cost-optimized prefactored high-order compact schemes, developed for shock-free error-bounded aeroacoustic applications, is presented. The cost-optimization theory of Pirozzoli (2007), based on the minimization of the computational cost for a given level of numerical error, is applied to obtain a new class of time-explicit prefactored compact schemes. Suitable high-order prefactored boundary closures, which are accurate and stable within a selected Fourier space envelope, are coupled with the new interior schemes. More conventional non-reflecting boundary conditions are shown to display an impedance mismatch, thus reducing the order of accuracy of the overall scheme. An eigenvalue analysis is performed, to verify the stability of the prefactored cost-optimized schemes coupled with the boundary closures. A parallelization strategy, based on a finite-sized overlapping interface, is presented, and weak scalability tests results are shown. Good agreement is shown between the predicted percentage cost-saving of the one-dimensional cost function and the measured savings in computational time for a one-dimensional monochromatic wave propagation test. Sample applications to broadband and two-dimensional space benchmark problems clearly highlight the favourable properties of the baseline scheme for large-scale aeroacoustic applications.
A Supermodular Generalized Nash Equilibrium Problem for Power Allocation in Cognitive Radio Systems

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The use of radio resources like Internet services and mobile phones has been growing rapidly in recent years, leading to inefficiency of the traditional assignment of the frequency band to the different communication systems. The use of Cognitive Radio systems allows a more flexible use of resources. In order to model the allocation of resources in a Cognitive Radio context, a Game-theoretical approach is efficient because it handles the radio resources like players which take their own decisions in a distributed way.

We discuss a Supermodular Generalized Nash Equilibrium Problem for power allocation in a Dynamic Spectrum Access context, characterized by the coexistence of primary and secondary users in the same frequency band. The secondary users are the true players of the game. We give mathematical conditions to be fulfilled in order to guarantee the existence and uniqueness of the Generalized Nash Equilibrium by making use of the property of supermodularity. The convergence of a Best Response-type algorithm to the Generalized Nash Equilibrium is also guaranteed.
The interaction of a uniform vortex with a pointwise one

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The motion of a uniform vortex in presence of a pointwise one is investigated. The fluid is assumed isochoric and inviscid and the flow planar. The shape of the uniform vortex is accounted for by means of the Schwarz function \( \Phi \) of its boundary. A novel theoretical approach \([1, 2]\) based on the evolution equation: \((\partial_t + U \partial_x)\Phi = \overline{U}\) is adopted, \(U\) and \(\overline{U}\) being the analytic continuations of the velocity and of its conjugate on the boundary. It leads to the integro-differential problem in the Schwarz function and in the point vortex position. The analytical solution of the above problem is faced by means of successive approximations. Results are compared with numerical simulations of the vortex motion.


We study the Darcy problem with lognormal permeability, which models the fluid flow in a bounded heterogeneous porous medium. We adopt a perturbation approach, expanding the solution in Taylor series with respect to the Gaussian random field.

The approximation properties of the Taylor polynomial are analyzed ([1,2]): we prove the local convergence of the Taylor polynomial to the solution, whereas, in general, the global convergence is not guaranteed. Nevertheless, for small values of the standard deviation of the random field, and small degree of the Taylor polynomial, the perturbation approach provides a good approximation of both the solution and its statistical moments.

The deterministic recursive problem solved by the expected value of the solution (first moment equation) is derived, analyzed and discretized with a full tensor product finite element technique. High order correlations between the derivatives of the solution and the random field are involved, which in the discrete setting are represented by high order tensors.

To overcome the curse of dimensionality, we search for the solution in low rank format, namely the Tensor Train format. An algorithm able to solve the recursive first moment problem in Tensor Train format is presented, and its effectiveness is shown on few numerical examples ([1]).


Vortex merging in relativistic flows

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In the present research the planar motion of an inviscid fluid (density $\rho$, pressure $p$ and enthalpy $h$) at relativistic velocities is considered. In light units, the conserved variables are $D = \rho w$, $S = Dw\mu u$ and $\tau = Dw\mu - D - p$, $w$ being the Lorentz factor, $u = (u_1, u_2)$ the velocity and $\mu = 1 + h$ the total specific enthalpy. The flow is described by a nonlinear hyperbolic differential system, so that it is explained in terms of wave propagation and interaction [1]. Among the flows in which the vorticity $\omega = -\partial_2 u_1 + \partial_1 u_2$ plays an important role, the merging between two initially uniform vortices will be investigated, by means of numerical integrations of the equations of motion [2,3].


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Active stress as a local regulator of global size in morphogenesis

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While a general consensus exists that the morphogenesis of living organisms has its roots in genetically encoded information, there is a big debate about the physical mechanisms that actually mediate its control. In embryo development, cells stop proliferating at homeostasis, a target state in terms of physical conditions that can represent, for instance, the shape and size of an organ. However, while control of mitosis is local, the spatial dimension of a tissue is a global information. How do single cells get aware of that at the same time? Which is their communication mechanism? While morphogen factors are demonstrated to play a key role in morphogenesis, and in particular for shape emergence, they seem unable to produce a global control on size by themselves and, conversely, many recent experiments suggest that active mechanics plays an important role. In our work we focus on a paradigmatic larval structure: the imaginal disc that will become wing in the fruit fly. By a formalization of theoretical conjectures in terms of simple mathematical models, we show that inhomogeneous stress, likely dictated by morphogenetic patterns, is an admissible mechanism to convey locally the global information of organ size.
Numerical Simulations of Self-Induced Thermodiffusion in Porous Media

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We consider a fluid-saturated porous medium exposed to a non-uniform temperature field, and describe it as a non-isothermal biphasic mixture comprising a solid and a two-constituent fluid. We model such a system by assuming that the fluid free energy density depends on the gradient of the solute mass fraction. This constitutive choice induces a coupling between the temperature gradient and the solute diffusive mass flux, which adds itself to the standard Soret effect.

We present numerical simulations of a thermogravitational cell [1] and thermohaline flows [2] to show how the modified constitutive framework, which is mandatory in diffuse-interface problems (c.f. Cahn-Hilliard model) [3], could be useful to emphasize some phenomenological features of the considered benchmarks, depending on their settings and characteristics.

References:


We study a non-isothermal binary fluid system by selecting the mass fraction of one of the two fluids as the order parameter of the system. We assume that the free energy of the system is of Cahn-Hilliard type, i.e. it features a term depending on the order parameter, which may be non-convex in this variable (when the fluids are partially miscible [2]), and a term depending on the gradient of the order parameter.

We determine a model in which the chosen free energy induces a spontaneous coupling between mass diffusion and thermal gradient. This coupling stems from the constitutive assumptions, rather than being a consequence of Onsager’s relations [1], and leads to a non-standard Soret effect, which adds itself to the standard one of thermodiffusion, if Onsager’s relations are invoked.

We present some implications of the non-standard Soret effect by discussing the outcomes of numerical simulations.

References:


Uncertainty quantification analysis in engineering design

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Nowadays the use of uncertainty quantification tools is mandatory when developing a new product, since they allow to monitor errors at each level and to control their propagation within the required tolerances.

The Monte Carlo simulation approach has a drawback: it requires a huge number of simulations, making the convergence slow when the number of parameters or dimensions increases, and this affects the possibility to introduce a new high quality product in the market.

Among all stochastic methods, in engineering the non-intrusive ones are more suitable, since it is not possible to modify kernels of well-known and strengthened commercial tools.

The Polynomial Chaos Expansion method is a good mathematical tool to perform this kind of analysis since it allows to drastically reduce the number of simulations and, consequently, the amount of computational time and resources. Furthermore, this method is suitable both for forward and backward analysis, allowing to get many information about variables distributions and the related statistics.

In this talk we propose the usage of the Polynomial Chaos Expansions method with Scilab as main tool to study the robustness of a simulation of an Organic Rankin Cycle system.

References:


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Compressed solving: a model reduction technique for PDEs based on compressed sensing

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We present a model reduction method for 1D advection-diffusion-reaction problems, motivated by the recent developments in the sparse representation field, and particularly by compressed sensing: namely, the CORSING (COMPressed SOLving) approach. The sparsity of the solution with respect to particular trial bases is exploited by a suitable choice of the test functions in the weak formulation, resulting in an underdetermined linear system (offline phase). Then, the solution is recovered using robust sparse optimization algorithms, like Basis Pursuit and Orthogonal Matching Pursuit (online phase). A Matlab implementation of the method, based on the toolboxes SPGL1 and OMP-Box, verifies the robustness and the reliability of the proposed strategy. A comparison with an SVD-based model reduction approach is provided. Finally, a preliminary generalization of the CORSING approach to the 2D case is applied to the classical Poisson problem.
Long-term structure-preserving numerical methods for Hamiltonian problems in Physics and Medicine

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It is the purpose of this talk to analyze the structure preservation properties of multi-value methods for the numerical solution of Hamiltonian problems, originating from Celestial Mechanics, Molecular Dynamics and Immunology.

In particular, we aim to achieve accurate and efficient numerical energy preservation and orbits computation in the dynamics of Solar system planets, by employing real data desumed by Nasa Horizons System, as well as numerical modeling of T-cell dynamics by discretization of suitable models arising from Mechanical Statistics is object of the investigations.

It is known that, in the spirit of numerical conservation of the invariants of Hamiltonian problems, the classical symplecticity property play a crucial role. However, only certain Runge-Kutta methods are candidate for symplecticity. Even if multivalue methods cannot be symplectic, it is possible to lead them possess a computationally cheap nearly preserving behavior through the properties of G-symplecticity, symmetry and zero-growth parameters for the parasitic components.

We are particularly interested in the long-time behavior of multi-value methods. Hence, we provide long-term error estimates by backward error analysis arguments, which permits to get sharp estimates for the parasitic solution components and for the error in the Hamiltonian. We prove that the effects of parasitism on the numerical solution are then negligible on time intervals of length $O(h^{-2})$, where $h$ is the stepsize of integration. The theoretical expectations are then confirmed by the numerical evidence.

References:


Irregularization accelerates iterative regularization

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When iterative methods are employed for the regularization of inverse problems, a main issue is the trade-off between smoothing effects and computation time, related to the convergence rate of iterations. Very often, the faster is the method the lower is the obtained accuracy. A new acceleration strategy is presented here, inspired by the choice of penalty terms formerly used in the context of Tikhonov regularization. More precisely, we define a correction term proposed by Huckle and Sedlacek in 2012 to enforce regularization capabilities, but with the opposite sign. This choice leads to an “irregularization” phenomenon, which speeds up the underlying basic method and can be controlled through a sequence of decreasing coefficients (as the iterations proceed, in order to prevent noise amplification) tuning the weight of the correction term. Filter factor expansion and convergence are analyzed in the simplified context of linear inverse problems in Hilbert spaces, by considering modified Landweber iterations as a case study.
Data assimilation: an ill posed problem
A Scalable Algorithm for Three Dimensional Variational Data Assimilation

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A research collaboration between us and CMCC (Centro Euro Mediterraneo per i Cambiamenti Climatici) give us the opportunity to use the Data Assimilation software called OceanVar [2]. OceanVar is based on a three dimensional variational scheme (3D-Var) and it is used in Italy to combine observational data (Sea level anomaly, sea-surface temperatures, etc.) with backgrounds produced by computational models of ocean currents for the Mediterranean Sea (namely, the NEMO framework), within the Mediterranean Forecasting System (MFS)[3]. Here, we present a scalable approach for variational DA: we introduce a decomposition of the global physical domain into sub domains. On these sub domains we define local 3D-Var functionals and we prove that the minimum of the global 3D-Var functional can be obtained by collecting the minimum of each local functional. The (global) regularization problem is decomposed into (local) regularization problems, in such a way. We perform a feasibility analysis of the related algorithm, analyzing its execution time and scalability [1]. Finally, our approach allows to tackle the ill conditioning of DA inverse and ill posed problem without reducing the number of available data furthermore, as discussed in [4].

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Variational Data assimilation in Computational Hemodynamics: Applications to Parameter Estimation

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With the progressive inclusion of numerical simulations in medical research and clinical practice, accuracy and reliability of patient-specific computational analyses need to be properly certified. This raises new challenges when estimating patient-specific parameters that may be too difficult or even impossible to measure in practice. Data assimilation techniques are required to merge available data and numerical models to assess the reliability of a quantitative analysis. In this talk, variational procedures will be considered to estimate (a) vascular compliance; (b) cardiac conductivities from available measures of vessel displacement and electric potential respectively. We pursue a constrained minimization approach based on the solution of the KKT system. In general, this leads to high computational costs, the constraint being represented by partial differential equations. Specific techniques for the sake of computational efficiency are mandatory. We will address using simplified models (like the Monodomain equations for electrocardiology) and surrogate modeling techniques like Proper Orthogonal Decomposition (POD), based on an on-line/off-line paradigm. We will illustrate successful experiences and pitfalls of this approach on the mentioned applications.
Data Assimilation of Anthropogenic Land Subsidence for the Compressibility Calibration in Productive Hydrocarbon Reservoirs

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Land subsidence is a major consequence of the pore pressure drawdown caused by fluid withdrawal from productive hydrocarbon reservoirs. Deep rock compaction induced by field depletion is measurable on the ground surface in terms of land displacements. In this study, an Ensemble Smoother (ES) data assimilation technique is developed in order to reduce the uncertainty on the constitutive parameters that characterize the geomechanical model. The procedure is tested for a real gas field seated at about 1500 m depth. The uniaxial vertical compressibility in virgin conditions and the ratio of the compressibility in loading/unloading have been calibrated as the most influential parameters in controlling the vertical land displacements. The ES in geomechanics appears to be a quite promising approach to reduce the compressibility uncertainty of the prior distribution by assimilating vertical displacements data. On the other hand, the ratio of the compressibility in loading/unloading conditions is not much influenced by the data assimilation, implying that the reservoir does not experience an important unloading.
Conditioning of Incremental Variational Data Assimilation

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Four-dimensional variational data assimilation (4D-Var) is a method for assimilating observations into a numerical model by minimising a weighted non-linear least-squares objective function which measures the error between the model forecast and the available observations. The problem is solved using an iterative optimisation algorithm. In practice an incremental version of 4D-Var is implemented in many operational forecasting centres, in which a sequence of linear approximations to the nonlinear least-squares problem is solved. This is equivalent to using an approximate Gauss-Newton method to solve the nonlinear minimisation problem.

The rate of convergence of the inner loop iteration scheme and the sensitivity of the analysis to perturbations are proportional to the condition number of the Hessian of the linear least-squares objective function. In this work we examine the conditioning of the variational assimilation method theoretically. We derive bounds on the condition number of the Hessian and use these examine the sensitivity of the conditioning to the length-scale in the
correlation structures and to the density and accuracy of the observations. Theoretical results are illustrated using a simplified system and the Met Office operational model. Finally we extend the bounds to the case where the model constraint is not enforced exactly.
Variational Ocean Data Assimilation for the Mediterranean Forecasting System

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The Mediterranean Forecasting System produces analyses for sea level, temperature, salinity and currents in the entire Mediterranean Sea. They are produced with a three dimensional variational assimilation scheme that considers both in situ and satellite data. The main characteristics of the data
assimilation scheme is the description of the background error covariance matrix with a series of matrix operators that subdivide the vertical and horizontal part of the error covariances and considers a fixed variability in the error covariance spatial and temporal scales. Results indicate the robustness of the data assimilation scheme for sparse in situ data and for dense satellite sampling data. Recently the temporal resolution of the error covariance matrix was changed to accommodate for higher temporal scale processes which can vary weekly and the results show improvements even if the spatial resolution is left to be coarse. Applications of the data assimilation scheme to Observing System Experiments for ARGO profiling float sampling strategies will be shown.
Numerical methods for inverse problems and image processing
Adaptive choice of the regularization parameter and matrix for the Arnoldi-Tikhonov methods

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Krylov subspace methods have always played a central role in the regularization of large-scale linear discrete inverse problems; among them, the Arnoldi-Tikhonov method [1] prescribes to project a Tikhonov-regularized problem into Krylov subspaces of increasing dimensions generated by the Arnoldi algorithm. If compared to a purely iterative method, the Arnoldi-Tikhonov strategy can theoretically deliver more accurate reconstructions, since some known features of the desired solutions can be easily enforced. However, to successfully apply the Arnoldi-Tikhonov method, a proper regularization parameter has to be chosen at each iteration of the Arnoldi algorithm, as well as an appropriate regularization matrix; furthermore, a reliable stopping criterion has to be considered.

The goal of our talk is to introduce two new parameter choice rules [3,4], based on some reformulations of the discrepancy principle, in order to adaptively set the regularization parameter; both these strategies are tailored to work in connection with the Arnoldi-Tikhonov methods, and the first one can simultaneously act as a stopping criterion, too. We also address the issue of choosing the regularization matrix, and we introduce two new strategies [2] that allow to approximate, into the Arnoldi-Tikhonov framework, regularization terms weighted in a generic norm.

We present the results of many meaningful numerical experiments regarding the application of the above mentioned schemes to image deblurring and denoising problems.


A method for constrained L1/TV image denoising

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Total Variation (TV) minimization is a very popular image denoising technique. When the noise degrading the image is impulsive, the data fidelity term is usually expressed in the $L^1$-norm, giving less importance to the so-called outliers. However, the non-differentiability of both the TV and the $L^1$-fitting causes numerical difficulties. In order to reduce these difficulties, we consider the constrained formulation of the L1/TV denoising problem where the TV has to be minimized under a constraint expressing $L^1$-data fidelity. The method we propose for the solution of this constrained problem generates a sequence of strictly feasible points. The search direction is obtained by inexactly solving a proximal Newton-type subproblem. A line-search globalization strategy is employed. The global convergence of the method can be proved. Numerical results show that the proposed approach is competitive with state-of-the-art L1/TV image denoising techniques in terms of both restored image quality and computational efficiency.
Inexact Bregman Regularization for astronomical images corrupted by Poisson noise

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The Bregman procedure is frequently employed in a contest of image restoration problems to obtain contrast enhancement ([1,2]). This procedure is an iterative scheme, where for each iteration it is required the computation of an exact solution of a minimization problem, i.e. a minimizer of a function. In most applications (in a image reconstruction framework) the computation of this exact solution is very expansive or, in some cases, impossible. In order to improve the efficiency of the method and contemporaneously to preserve the convergence and the features of the Bregman iterative procedure an inexact version of this scheme is proposed, where the inexactness of the inner subproblems’ solution is kept under control by the introduction of a new stopping criterion. Moreover, this procedure allows to obtain accurate reconstruction when an overestimation of the regularization parameter is known. This is convenient when the data are corrupted by Poisson noise, since it makes possible to use the most advanced techniques and algorithms for minimizing the general Kullbach-Leibler divergence combined with a regularization term. Numerical results are presented in order to evaluate the efficiency of the Inexact Bregman iterative scheme, in a contest of image restoration, considering deblurring and denoising problems. A practical application is presented in an astronomical framework ([3]), in deconvolution problems of high contrast images consisting of very bright stars and smooth structures underlying the stars, structures which don’t permit accurate reconstructions with classical deblurring algorithms.


Levenberg-Marquadt and Adaptive Quadratic Regularized methods for ill-posed nonlinear systems

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In this talk we will analyse a class of algorithms for ill-posed nonlinear systems, which includes Levenberg-Marquadt [3] approaches as well as Adaptive Quadratic Regularized (ARQ) methods. ARQ methods employ a model consisting of the Euclidean residual regularized by a quadratic term [1,4]. Local and global convergence properties of ARQ approaches for well-posed nonlinear systems have been extensively studied [1,2]. Here, we will show that suitable modifications of these methods give rise to regularizing methods for ill-posed problems. The noise-free case as well as the realistic situation where noisy data are given will be considered. We will further show that in the noise free case properly chosen regularizing terms also provide global convergent procedures. At this regard, we remark that global convergence of regularizing approaches for ill-posed problems is still an open task.


Unsupervised tissue segmentation and classification of three-dimensional 3T prostate MRSI data by hierarchical non-negative matrix factorization for automatic tumour detection and visualisation

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A non-negative blind source separation technique, known as non-negative matrix factorization (NMF), is hierarchically applied to three-dimensional 3T MRSI prostate data to extract characteristic patterns for tumour and benign tissue, and to visualise their spatial distribution. Since several NMF algorithms are available in the literature, in this study three different NMF implementations are considered and embedded into the same kind of hierarchical scheme, which allows to automatically retrieve the patterns of interest and to provide a tissue characterisation of the given MRSI data. Extensive simulation and in vivo studies show that the hierarchical scheme provides
higher quality tissue patterns compared to those ones obtained by performing only one NMF level. Furthermore, the three implementations perform similarly, although the one known as CONVEX-NMF provides a more reliable tumour pattern when the MRSI data set is characterised by moderately aggressive tumour spectra.
Many efforts to generalize the conjugate gradient method to non-quadratic functionals have been made in the recent literature, both in Hilbert and Banach spaces. Here we propose a generalization of the conjugate gradient method for the minimization of a p-norm cost functional $\Phi(x) = ||Ax - y||_p^p$, related to the solution of the operator equation $Ax = y$, where $A : X \to Y$ is a linear operator between $L^p$ Banach spaces. It is well known that the new “geometry” of the $L^p$ spaces, for values of the constant $1 < p < 2$, can substantially reduce the over-smoothness effects of any iterative restoration process in $L^2$ Euclidean space [1]. The high convergence speed of conventional conjugate gradient in $L^2$ Hilbert space gives rise to a fast minimization method in $L^p$ Banach spaces too.

The algorithm is applied to enhance the spatial resolution of microwave radiometer data. The problem which describes the relationship between the coarse but partially correlated measurements and the brightness temperature belongs to the class of Fredholm integral equation of the first kind.
On the application of spectral projected gradient methods in image segmentation*

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Image segmentation, as many problems in image processing, can be addressed via the optimization of a cost functional. We consider a convex relaxation of Chan-Vese’s active contour model [2]. In this case, the optimization problem takes the form

\[
\min_{u,c_1,c_2} E_1(\nabla u) + \lambda E_2(u, c_1, c_2)
\]

s.t. \(0 \leq u \leq 1\),

(1)

where \(u\) is a continuously differentiable function related to the segmented image, \(c_1\) and \(c_2\) are the mean intensity values of the objects and background of the image, \(E_1\) is a regularization term, \(E_2\) is a fidelity term measuring in some sense the distance between the given image and a two-phase image with intensities \(c_1\) and \(c_2\), and \(\lambda\) is a positive parameter. A standard approach to solve this problem consists in alternating the minimization with respect to \(u\) and \((c_1,c_2)\); the latter minimization can be performed exactly, by expressing \(c_1\) and \(c_2\) as functions of \(u\). We solve problem (1) by using a different approach, based on a nonmonotone spectral projected gradient method [1], where the minimization is carried out with respect to all variables, but the steplength selection procedure is performed by taking \(c_1\) and \(c_2\) fixed. Numerical experiments show the effectiveness of our strategy.

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Optimization methods for large-scale deconvolution on HPC architectures with applications in Microscopy

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A number of modern imaging applications require deconvolution techniques to improve reconstruction accuracy by mitigating the distortion effects caused on the data by the acquisition system. This can be computationally demanding, mainly in the case of large-scale problems. In this talk we present an effective deconvolution approach based on an accelerated gradient method, which is also able to exploit the power of some modern HPC architectures. The accelerated deconvolution algorithm is developed on the basis of scaled gradient projection (SGP) method [1], which is particularly suitable for the solution of constrained optimization problems coming from the maximum likelihood approach and, for the regularized version, by the maximum a posteriori approach. Advances on the use a new steplength selection rules based on Ritz coefficients will be also discussed. These rules were recently proposed by R. Fletcher in the unconstrained context [2]. Some meaningful numerical experiments on large-scale 2D and 3D microscopy data will show the benefits of the proposed approach and how it is able to exploit GPU architectures.

New developments and applications of Groebner bases
Applications of Groebner bases to simple graphs

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Classes of simple graphs are studied using computational and algebraic methods in order to give geometrical models in real connection problems. Let $G$ be a simple graph. An algebraic object attached to $G$ is the edge ideal $I(G)$ which is a monomial ideal of the polynomial ring in $n$ variables, where $n$ is the number of vertices of $G$ ([6]).

We investigate algebraic properties of edge ideals via Groebner bases. More precisely, we use the theory of Groebner bases to characterize monomial $s$-sequences that arise from $G$. We introduce some classes of acyclic graphs for which, using the Gröbner bases, we show that necessary and sufficient conditions hold in order that their edge ideals are generated by $s$-sequences. Moreover we establish a condition for which a monomial sequence of generators associated to the edge ideal of a forest is an $s$-sequence ([2], [3], [4]).

The notion of $s$-sequence is employed to compute algebraic invariants of the symmetric algebra associated to $I(G)$ such as the dimension, the multiplicity and the Castelnuovo-Mumford regularity ([1], [5]).


Graphs of paths and associated monomial algebras

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We consider two classes of complete bipartite graphs of paths, studied in [2], with good algebraic properties. They are described by ideals of mixed products $L = I_rJ_s$ and $L' = I_rJ_{s-1} + I_{r-1}J_s$, in two sets of variables in the polynomial ring $K[X_1, \ldots, X_n; Y_1, \ldots, Y_m]$, over the field $K$, where $I_r$ is the $r$-th squarefree Veronese ideal in $K[X_1, \ldots, X_n]$ and $J_s$ is the $s$-th squarefree Veronese ideal in $K[Y_1, \ldots, Y_m]$. We consider the case $r = s = 2$ and we describe phenomena that can be modeled by such graphs. The associated monomial algebras $K[L]$ and $K[L']$ are algebras of Segre-Veronese type that can be intensively studied using the Groebner bases theory.


Which Principal Borel ideals are Gotzmann?

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In this talk, I’ll present a joint work with S. Eliahou entitled Which principal Borel ideals are Gotzmann? It is linked with papers [2] and [1] presented to SIMAI Congress in 2006. We denote by $S_n$ the set of monomials in $n$ variables, and by $S_{n,d}$ those monomials in $S_n$ of degree $d$. For $u \in S_{n,d}$, we denote by $\langle u \rangle$ the principal Borel ideal generated by $u$. We say that $u$ is a Gotzmann monomial in $S_n$ if the set $\langle u \rangle$ is a Gotzmann ideal in $S_n$. Let $u \in S_n$, we denote by $\gamma_n(u)$ the smallest exponent $k \in \mathbb{N}$ such that $ux_n^k$ is Gotzmann. We focus here on Gotzmann monomials in $S_n$ for $n$ small. For $n = 3$, we obtain a complete answer for the function $\gamma_n(u)$ and for $n = 4$, we present a general conjecture.

References:


**Algebraic and geometric models for business**

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In integer programming the classical transportation problem TP describes the exchange among $n$ factories $F_1, \ldots, F_n$ which produce a respective supply of $U_1, \ldots, U_n$ units of an indivisible good and $m$ stores $S_1, \ldots, S_m$ which have respective demands of $V_1, \ldots, V_m$ units. TP is modelized by the algebraic-geometric (1-1) Segre-model, given by a semigroup homomorphism $\pi$, or by a $k$-algebra homomorphism $h$ that lifts $\pi$, constructed by the Segre product of two polynomial rings on a field $k$ (i.e the real number field $R$) in $n$ and $m$ variables respectively. In this research we improve the classical model TP and we propose a new algebraic-geometric model called (1-2) Segre-Veronese model for describing the exchange among the $n$ factories and the $\binom{m}{2}$ groups of 2 stores, coming by the aggregations of the $m$ stores. The enumeration problem for elements of a fiber of $\pi$ with moderate size can be solved using Groebner bases theory.


On the Birkhoff model for ranking problems

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The problem of ranking a number of alternatives based on scores or preferences assigned by multiple voters (or under multiple criteria) has become exceptionally important in modern applications. In addition to well-known examples such as rankings of colleges, sport teams, stocks, or webpages, ranking methodologies have been used in novel surprising ways. Concerning the mathematical tools, let $S_n := \text{the symmetric group of the set of data } \{1, 2, ..., n\} = [n]$, of cardinality $n!$ and let $\pi \in S_n$ any permutation.

Let $S = K[X_\pi, \pi \in S_n]$ the polynomial ring with variables indexed by permutations in $S_n$, whose coefficients are in any infinite field $K$ of characteristic zero (the field of real numbers $\mathbb{R}$).

Let $T = K[Y_1, Y_2, ..., Y_n]$ a polynomial ring, where the indeterminates are viewed as a system of parameters.

Definition: A STATISTICAL RANKING MODULE is an homomorphism $f : S \rightarrow T$.

The BIRKHOFF MODEL studies SAMPLING PROBLEMS FROM STATISTIC.

The homomorphism $f : S \rightarrow T$ is such that $T = K[Y_{ij}, 1 \leq i \leq j \leq n]$, where $Y_{ij}$ is the entry of a generic matrix and $f(x_\pi) = \prod Y_{i,\pi(i)}$

RESULTS: Our results concern the Birkhoff ranking model for subsets of the full set of permutations.

Many objects of convex geometry and geometric combinatoric appear in products of art. We define a simplicial complex on a vertex set \( \{1, 2, \ldots, n\} \) and a convex polytope on set of points \( \{v_1, \ldots, v_m\} \) of \( \mathbb{R}^n \), from the point of view of commutative algebra and polyhedral geometry. By using the Groebner bases theory, we obtain new simplicial complexes and new polytopes, that could be interesting subject of the art. More precisely, we introduce a term order \( < \) on the monomials of the polynomial ring \( K[X_1, \ldots, X_n] \), \( K \) a field, and for special classes of binomial ideals we determine their initial complex, hence the convex polytope. We recovery them in products of art as painting and sculpture during the XX-XXI centuries (see the Dalì hypercube).

Complex Systems
(SisCo-SIMAI Activity Group)
Modeling altruism and selfishness in welfare dynamics

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Social systems need to be viewed as complex evolutive systems, including nonlinear interactions and learning phenomena, where collective comportment appear and appropriate mathematical structures suitable to catch these features are needed. In this talk a mathematical structure is proposed modeling welfare dynamics in societies viewed as complex evolutive systems subject to different policies of wealth distribution [1]. Interactions among agents are modeled as stochastic games triggered by a threshold. The approach contains the whole path from modeling to simulations, through a qualitative analysis of the initial value problem. Simulations are developed to put in evidence by visualization the dynamical behavior of the following features:

• Influence of the dynamics of the threshold $\mu$ on the trend, asymptotic in time, of the solutions, by comparison with the case of constant threshold.

• Influence of the initial conditions by understanding how the dynamics differ depending on the initial distribution of wealth; for instance by comparing the dynamics of a population where the initial conditions are concentrated on poor classes to that of a population characterized by a higher presence of wealthy classes.

• Interplay between the influence of $\mu$ and that of the initial conditions.

• Rôle of a "selfishness" parameter $\gamma$.

A kinetic approach to traffic flow on road networks

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This talk deals with a new kinetic model describing traffic flows on networks of different interconnected roads. According to the author’s knowledge, this is the first attempt to model such system by means of kinetic equations.

The idea is to use the generalized kinetic and stochastic game theory of active particles together with discrete representation of the microscopic states of vehicles. This way the model successfully captures both the implicit stochasticity of human behaviors, hence ultimately of microscopic car interactions, and the intrinsic microscopic granularity of the distribution of vehicles along a road, which indeed do not properly form a continuum even in congested situations.

More precisely, we present the modeling of two basic types of junctions: a junction with one incoming and two outgoing roads, which introduces the concept of flow distribution and the dual junction with two incoming and outcoming road which introduce the concept of right of way.

Finally, we show some numerical simulations and we discuss a qualitative analysis of the initial/boundary value problem on such networks.
Nonlocal interaction equations with two species

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We present a systematic existence and uniqueness theory of weak measure solutions for systems of nonlocal interaction PDEs with two species, which are the PDE counterpart of systems of deterministic interacting particles with two species, see [3]. The main motivations behind those models arise in cell biology, pedestrian movements, and opinion formation. In case of symmetrizable systems (i.e. with cross-interaction potentials one multiple of the other), we provide a complete existence and uniqueness theory within (a suitable generalization of) the Wasserstein gradient flow theory in [1], which allows to consider interaction potentials with discontinuous gradient at the origin, see [2]. In the general case of non-symmetrizable systems, we provide an existence result for measure solutions which uses a implicit-explicit version of the JKO scheme, which holds in a reasonable non-smooth setting for the interaction potentials. Uniqueness in the non symmetrizable case is proven for smooth potentials using a variant of the method of characteristics. One-dimensional local nonlinear stability for a nonlocal predator-prey model is discussed, both at particles and PDE levels providing some numerical results.


A Kinetic Model of Crowd Evacuation from Bounded Domains

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The presentation is based on [1], in which we propose a kinetic model for the evacuation of crowds from bounded domains, such as a room with one or more exit doors. We use a hybrid representation of the crowd, with continuous-discrete features, that is position is assumed to be a continuous variable, while velocity direction is a discrete variable.

The modeling approach considers dynamics caused by interactions of walking people at the micro-scale with all the other pedestrians and with the geometry of the domain (i.e. position of walls and of exit doors). Interactions are non-local and trigger a decision process which modifies the velocity direction of people in a stochastic manner, whereas for simplicity the velocity modulus is assumed to depend deterministically on the local density.

Numerical simulations are developed to study evacuation time depending on the size of the exit zone, on the initial distribution of the crowd and on a parameter which weighs the unconscious attraction of the stream and the search for less crowded walking directions.

An Easy-to-Use Approach for Simulating Traffic Flow on Networks

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In this talk we present a model for traffic flow on networks based on a hyperbolic system of conservation laws with discontinuous flux. Each equation describes the density evolution of vehicles having a common path along the network. We consider a Godunov-based approximation scheme for the system which exhibits surprising properties, being able to select automatically a reasonable solution without requiring external procedures at junctions (e.g., maximization of the flux via a Linear Programming method [2,4]). Since users do not have to deal with vehicle dynamics at junction, the numerical code can be implemented in minutes.

We also show how the scheme can be recast in the framework of the classical theory of traffic flow on networks, where a conservation law has to be solved on each arc of the network. This is achieved by deducing a modified analytical problem which is correctly solved by the numerical algorithm. Numerical comparisons with standard schemes [2,4] are also presented.

Reference papers are [1,3].


Some remarks on the risk driving index definition: mathematical models

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Beginning from well-known model of traffic we add another equation which represents some aspects of safety driving. This equation can be or a PDE or a suitable equation based on the generalized kinetic theory for active particles, in which short range interactions among drivers are modeled as stochastic games. Our analysis considers two different parts: objective and subjective. Namely, the objective part concerns an analysis of the driving conditions which do not depend on the driver and the subjective part regards the physical and psychological conditions of the driver. Of course, when an individual drives he is liable to both parts. We wish to introduce some considerations in order to define a risk driving index (or, in symmetric way, a safe driving index). This index could be utilized as tool for the governance of vehicular traffic, with regard both the intrinsic difficulty of the road course, the weather conditions and the state of a driver. In other words, we propose a measure which enables to establish when a road can be covered with a degree of care. We give also an attempt of data validation.
Kinetic description of optimal control problems and applications to consensus modeling

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In this talk we will discuss an optimal control problem for a large system of interacting agents using a kinetic perspective. As a prototype we first introduce a microscopic model of consensus formation under constraints. In order to investigated the mean–field description of this problem, we propose a Boltzmann-type equation based on a model predictive control formulation. In particular, the receding horizon strategy allows to embed the minimization of suitable cost functional into binary particle interactions acting as instantaneous control. We derive the corresponding Fokker-Planck asymptotic limit of the consensus dynamic and we show that stationary solutions can be computed explicitly. Finally we report several numerical results showing the robustness of the present approach.
On the Modeling of Learning Dynamics in Large Living Systems

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Our presentation deals with the modeling of learning dynamics in a large system of interacting entities. The mathematical approach is based on the kinetic theory of active particles. Their microscopic state is modeled by a scalar variable called activity, which is assumed to be heterogeneously distributed among the particles. Nonlinear interactions lead to collective phenomena of learning. The structure allows the derivation of specific models and of numerical simulations related to real systems. The leading idea proposed in this theory is that individuals learn by interactions, whose frequency depends on a suitable metric distance. The learning process is characterized by nonlinear interactions among individuals. We introduce the reference mathematical structure, discuss existence and uniqueness properties of the solution of the initial value problem in a suitable functional space and then discuss a practical examples constructing the so called table of games and showing the results of the related numerical simulations.
On a Model of Darwinian Dynamics and Competition between Tumor and Immune Cells

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The talk concerns the modeling of the early stage of cancer phenomena, namely mutations, onset, progression of cancer cells, and their competition with the immune system. The mathematical approach is based on the kinetic theory of active particles developed to describe the dynamics of large systems of interacting cells, called active particles. Their microscopic state is modeled by a scalar variable which expresses the main biological function. The modeling focuses on an interpretation of the immune-hallmarks of cancer.


Transient states and congestion in traffic dynamical models on road networks

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The complex networks have been extensively used to cope with the problem of extracting relevant information from the big data-base that new technologies allow to collect on complex systems. Biological systems, social systems and economics are the main application research fields. Statistical Physics has developed suitable methods to characterize the equilibrium or states and the existence of phase transitions. Recently the data base have been enriched by dynamical properties of the considered systems opening the possibility of studying the transient states and the transitions to critical states under a dynamical point of view. As a consequence there has been new motivations to study stochastic dynamical systems on network-like interactions structures. Being inspired by the traffic dynamics we propose a class of models defined on a network topology whose nodes are characterize by a state \( x \in [0,1] \) which evolves according

\[
\dot{x}_k = \sum_j \pi_{kj}(t)\Phi(x_j, x_k) - \sum_k \pi_{jk}(t)\Phi(x_k, x_j)
\]

where \( \pi_{kj} \in [0,1] \) is a stochastic random matrix which defines the weights of the network links (i.e. \( \pi_{kj} \) weights the directed link between the nodes \( j \) and \( k \) and \( \sum_k \pi_{kj} = 1 \)). The functions \( \Phi(n_j, n_k) \) define the 'particles' flows on the link \( j \rightarrow k \) which is a nonlinear function of the node states (and possible of the node features) and satisfies the conditions

\[
\phi(0, x_k) = 0 \quad \lim_{x_k \to 1} \phi(x_j, x_k) = 0 \quad \lim_{x_j \to 1} \phi(x_j, x_k) \geq 0
\]
and for any value $x_k$ there exists a critical point such that $\partial \phi / \partial x_j = 0$, which corresponds to a local maximum for the $x_j$ state. According to our assumptions when the state of a node tends to 1, the node is congested and it prevents other particles from entering in the node. This gives rise to a congestion spreading in the network following a backward cascade. We have studied the existence of equilibrium points for the average dynamics and their stability, the transition probabilities to congested states and the statistics of the first congestion time and the effect of a delay time for the propagation of the information on the network on the dynamics in congested states. We have also considered possible local strategies to control the congestion development and the congestion spreading in the system. These results have been applied to the study of traffic congestion formation on a road network using the traffic data recorded by 300 magnetic spires in the road network of Emilia Romagna region in Italy. This system allows to record microscopic information on vehicle dynamics (transit time and velocity) on the main road network covering an area of order 20000 km$^2$. The theoretical model suggests the existence of new observables that may forecast the development of traffic congestion.
A 2-population kinetic model for vehicular traffic

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In the study of vehicular traffic we measure quantities like density, flux and average speed experimentally. However, the diagrams that relate these variables can have different interpretations. Starting from a model of vehicular traffic, based on kinetic theory, in which the space of microscopic velocity is discrete, we try to understand the nature of experimental diagrams. Although the models with 1-population provide an equilibrium curve that reflects the characteristics of traffic, the real data seem to suggest a dependence of the asymptotic distribution on the initial one. Extending the model to 2-population, we can show that we obtain the scattering of real data if we consider the presence of vehicles with mixed features (like average length and maximum speed): what has been suggested as a result of stochastic human behavior, seems predicted in a deterministic way.


Mathematical Models and Computational Methods in Biomedicine
Compartmental Models for Nuclear Medicine Data: an Inverse Problems Perspective

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Compartmental analysis is a computational tool for the modeling of nuclear medicine data that, in its most recent applications, exploits spatio-temporal information provided by Positron Emission Tomography (PET). This talk introduces two novel compartmental models describing the excretion of 18Fluoro-deoxyglucose (FDG) in the renal and hepatic systems. The first model accounts for variations in FDG concentration due to water reabsorption in renal tubules and for increase of bladder’s volume during the excretion process. The second model accounts for the dual blood supply proper of the liver circulatory system and uses tracer concentration in the gut to describe the flow in the portal vein at the liver entrance. The computational reduction of both models is performed by using inverse problems techniques: in the first case we used a non-stationary steepest descent approach that explicitly accounts for the Poisson nature of nuclear medicine data; in the second case, a regularized multi-dimensional Newton algorithm with an ad hoc rule for the optimal selection of the regularization parameter. The applications considered illustrate new insights about the role of metformin in cancer metabolism and utilizes data recorded by a PET system for small animal models.
The determination of a protein’s scale size is a difficult problem that is typically addressed by means of crystallography. Small angle X-ray scattering (SAXS) may offer an alternative approach, which does not require the availability of a crystalline sample. Further, SAXS allows dynamic measurements and provides access to information not limited to the surface of the sample, being able to measure inside the material without sophisticated sample preparation. A SAXS experiment typically produces a one-dimensional scattering intensity obtained by circular averaging the two-dimensional scattering pattern observed in the experiment. In order to determine the size information from this intensity, one needs to solve an ill-posed inverse scattering problem. This talk briefly introduces the SAXS modeling under the assumption that all nanoparticles in the system of interest are equally sized and shaped, and presents a statistical method to determine the size of the nanoparticles. SAXS data are obtained by an azimuthal regrouping of scattered photons acquired by a charged coupled device and therefore are Poisson distributed. The talk will show the effectiveness of Expectation Maximization, when coupled with an appropriate stopping rule, to retrieve positive parameters from SAXS data.
The Hough Transform and a Novel Prognostic Index for Chronic Leukemia

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It has been recently proved that a computational analysis of Positron Emission Tomography/Computerized Tomography (PET/CT) images allows the assessment of alteration of bone structure and bone marrow metabolism in adult patients with advanced chronic lymphocytic leukemia and that this kind of analysis may even offer prognostic potentials [2]. The crucial requirement for the reliability of this study is the application of a pattern recognition method able to accurately segment the intra-bone space in clinical CT images of the human skeleton. The talk shows how this task can be accomplished by a procedure based on the definition of Hough Transform for special classes of algebraic curves [1]. The idea is the one to introduce a catalogue of curves that satisfy some specific algebraic geometry conditions, to compute their Hough Transform and apply a standard recognition approach based on the optimization of an accumulator function. The effectiveness of this method will be proved against low-resolution clinical CT data and lead to the recognition of complex profiles in many different districts of the human skeleton.

Sequential Monte Carlo Samplers for the
determination of neural activity from
neurophysiological data

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Magnetoencephalography records non-invasively the magnetic fields produced by the brain. In the dipolar approximation, the neural current is modeled as an unknown number of point sources, termed current dipoles. We consider the problem of estimating the number of dipoles, their locations and strength, from a single spatial distribution of magnetic field. We use a Bayesian approach, with uninformative priors for all parameters but the number of sources, which is assigned a Poisson prior with low mean. We set up a sequential Monte Carlo sampler, that samples from a tempering sequence (a one-parameter family) of distributions, that closely reminds the regularization path. From the so-obtained posterior distribution we compute point estimates of the source parameters. Simulated data show very good localization properties, and experimental data evoked by somato-sensory stimulation confirm that the method can localize sources in real scenarios.

New Perspectives on Applicabilities in Graph Theory
Graphs & Neuro-Fuzzy Approaches to Solve Inverse Problems in Non Destructing Testing and Evaluation

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Non-Destructive Testing in the eld of defects identication in metallic elements plays a remarkable role with special regard to those sectors where the integrity of the material is strictly required. As a consequence, the detection of defects and discontinuous deformations in metallic plates and bars, together with the relevant shape classication, provides to the operator useful information on the actual mechanical integrity of the specimen [1]. When transformations are being studied, the loss of uniqueness in the solution, together with the relevant fragmentation of the strain elds inside the solid can be observed, the equilibrium coming out as a solution presented from a ne mixture among phases. In this context, starting from a theoretical characterization of physical models with respect to computational aspects, a comparison with data from experimental investigation based on eddy current technology is carried out. Finally, a new approach by neuro-fuzzy inference system exploiting a network structure represented by graphs is proposed to solve the inverse problem. In particular, Mamdani and Sugeno fuzzy inference systems and fuzzy similarities [2], [3] have been exploited to investigate any discontinuities of the specimen subject to plastic deformation obtaining a map of mechanical stress (not obtainable by measurement campaign) calculated by application of the constitutive laws.


Vertex covering optimization in Veronese bi-type graph ideals

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In [1], [5] monomial ideals of the ring $R = K[X_1, \ldots, X_n; Y_1, \ldots, Y_m]$ were introduced and their link with bipartite graphs was studied. We deal with ideals of Veronese bi-type, namely monomial ideals of $R$ generated in the same degree: $L_{q,s} = \sum_{k+r=q} I_{k,s}J_{r,s}$, with $k, r \geq 1$, $s \leq q$, where $I_{k,s}$ is the ideal of Veronese type generated on degree $k$ by the set \{ $X_a^{a_i_1} \cdots X_a^{a_in}$ | $\sum_{j=1}^n a_{ij} = k$, $0 \leq a_{ij} \leq s$, $s \in \{1, \ldots, k\}$ \} and $J_{r,s}$ is the ideal of Veronese type generated on degree $r$ by \{ $Y_b^{b_i_1} \cdots Y_b^{b_im}$ | $\sum_{j=1}^m b_{ij} = r$, $0 \leq b_{ij} \leq s$, $s \in \{1, \ldots, r\}$ \}.

For $s = 2$ and $q \geq 3$, the ideals $L_{q,2}$ are associated to the walks of length $q-1$ of complete bipartite graphs having loops in all their vertices $x_1, \ldots, x_n, y_1, \ldots, y_m$, the so-called strong quasi-bipartite graphs $K'_{n,m}$, and correspond to the generalized graph ideals $I_q(K'_{n,m})$.

The ideals of Veronese bi-type $L_{q,2}$ can be considered as bi-polymatroidal ideals in $R$ that derive from a special class of discrete bi-polymatroids, namely monomial ideals generated in a single degree such that for any two minimal generators $u, v$ with $\deg_{X_j}(u) > \deg_{X_j}(v)$ or $\deg_{Y_k}(u) > \deg_{Y_k}(v)$ there exist $j \in [n]$ with $\deg_{X_j}(u) < \deg_{X_j}(v)$ or $l \in [m]$ with $\deg_{Y_l}(u) < \deg_{Y_l}(v)$ for which $X_j(u/X_i)$ or $Y_l(u/Y_k)$ are minimal generators.

Algebraic properties, such as the monomial localization of the bi-polymatroidal ideal $I_q(K'_{n,m})$, are examined in [3]. It is also pointed out an algebraic aspect concerning a generalization of the notion of minimal vertex covers, given in [2], [4], [6], that is the ideal of vertex covers for the generalized graph ideal of $K'_{n,m}$. Such ideal, denoted by $(I_q)_c(K'_{n,m})$, is generated by all monomials $X_{i_1} \cdots X_{i_k} Y_{j_1} \cdots Y_{j_h}$ such that $(X_{i_1}, \ldots, X_{i_k}, Y_{j_1}, \ldots, Y_{j_h})$ is an associated

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prime ideal of $I_q(K_{n,m}')$. Finally, the structure of $(I_q)_c(K_{n,m}')$, $n \geq m$, is fully described. The study of all these facts is devoted to find specific useful tools for improving actual critical situations for the connections in the field of communications and transport.

1. Imbesi, M. and La Barbiera, M. 2013 *Algebraic properties of non-squarefree graph ideals*. Math. Reports, 65(15), 107–113


3. Imbesi, M. and La Barbiera, M. *On algebraic properties of Veronese bi-type ideals arising from graphs*. Submitted


Our attention is fixed to a simply graph $G_3$ of paths of length 2 of a complete graph $G_3$ on a vertex set $\{1, 2, ..., n\}$ that can be employed to modelise different fields of the life. More precisely we consider the polynomial ring $A = K[X_1, X_2, ..., X_n]$, $K$ a field, and the monomial squarefree ideal $I_3$ of $A$, generated by \( \binom{n}{3} \) monomials $X_{i_1}X_{i_2}X_{i_3}, 1 \leq i_1 < i_2 < i_3 \leq n$, so called 3-Veronese square free ideal of $A$. For a bounded set of variables, we study:

1. The monomial algebra $K[G_3] = K[T_{ijk}, 1 \leq i \leq j \leq k \leq n]$
2. The Groebner basis of the presentation ideal $J_3$ of $K[G_3]$
3. Algebraic invariants of $K[G_3]$

In particular we study for a bounded set of variables, all possible monomial orders on $K[T_{ijk}, 1 \leq i \leq j \leq k \leq n]$ that give a quadratic binomial Groebner basis for $J_3$.

Theorem: There exists a term order $<$ on $K[T_{ijk}, 1 \leq i \leq j \leq k \leq n]$ such that the sorted monomials are precisely the $< -$ standard monomials modulo $J_3$. The initial ideal $\text{in}_<(J_3)$ is generated by square free monomials. Theorem

In the second part of the talk we consider an application of obtained results to problems of traffic, where many graphs of the type introduced before naturally arise, when some corners of the streets are without obstacles.

On Ideals Associated to Complete Bipartite Graphs

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It is known that graphs are useful symbolic representations for several connection problems. We consider complete bipartite graphs, $K_{n,m}$, and we study good properties for the generalized graph ideals $I_q(K_{n,m})$. These ideals are monomial ideals in two sets of variables generated by square-free monomials of fixed degree $q$, associated to the paths of length $q - 1$ of $K_{n,m}$. In particular, they are ideals of mixed products and various results about them are known [3], [4]. However, some problems arise when we want to study algebraic and geometric properties for them and for some algebras related to them [1], [2]. Using computational and algebraic methods, we investigate on $I_q(K_{n,m})$, in order to study when they have a linear resolution, and to compute standard invariants for the symmetric algebra $Sym(I_q(K_{n,m}))$. Moreover, the structure of minimal vertex cover of $I_q(K_{n,m})$ is fully described.


Numerical methods for coupled problems
ELECTROMECHANICAL MODELLING AND 
IN SILICO ANALYSIS OF A RAT CARDIAC 
SYNCYTUM

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We performed a study on the mechanics and electrophysiology occurring during the contraction of a 2D syncytium made of rat cardiomyocytes by carrying out numerical simulations of an electromechanical model for its cell and tissue components. From the online database CellML 1.1 we took three different models describing rat ventricular phenomena at the cell scale, which had already been corrected and integrated into the so-called PHN (Pandit-Hinch-Niederer) model: Pandit et al. electrical activity model [8], Hinch et al. calcium dynamics model [3] and Niederer et al. active tension (or contraction force) generation model [7]. Then, in order to simulate the electromechanical response of our 2D sheet of cardiac tissue, we added a Monodomain model [1] to allow the propagation of the action potential and a quasi-static finite elastic model [4][9] to simulate the biomechanical response at the tissue scale. The discretization of the complete model was achieved by using finite elements in space and semi-implicit finite differences in time. At last we performed a set of simulations changing the values of some relevant parameters in order to match the experimental results found in the literature [2][5][6].


Interface Control Domain Decomposition (ICDD) Method for Stokes Darcy coupling

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We present the Interface Control Domain Decomposition (ICDD) method to address heterogeneous and multiphysics problems by overlapping subdomain splitting. Interface controls are unknown functions used as Dirichlet boundary data on the interfaces of an overlapping decomposition designed for solving boundary value problems. The controls are computed through an optimal control problem with interface observation [1], [2]. The main advantage of applying this approach to heterogeneous problems is to avoid sharp interfaces which would require an in depth knowledge of the local physical behavior (interface conditions) of the specific problem. In this talk we consider the Stokes/Darcy problem modeling the filtration of incompressible fluids through porous media, aiming at discussing both theoretical and computational aspects of the ICDD method, as well as at comparing this approach with classic coupling techniques based on the Beavers-Joseph-Saffman interface conditions [3].


Finite elements for Immersed Boundary Method

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The finite element method has been applied with success to the Immersed Boundary Method, for the numerical treatment of fluid-structure interaction problems [2] [1]. Recently a new variational formulation based on the introduction of a Lagrange multiplier has been introduced. We show under reasonable assumptions that the scheme results to be inconditionally stable with respect to the time discretization.


We present a numerical method to simulate the movement of a thin inextensible beam immersed in an incompressible viscous fluid. Our approach combines the flexibility of mesh moving/front tracking techniques with an additional level set description of the interface. The computational mesh is automatically aligned to the interface by minimizing a nonlinear, constrained functional [1]. This optimization based mesh adjustment does not change the topology of the mesh while guaranteeing optimal mesh quality. Due to the mesh alignment, discontinuities of the solution variables (pressure) across the interface can be captured accurately. This approach allows for very large structural displacements. To solve the fluid-structure interaction problem, we adopt the classical Dirichlet-Neumann method with an acceleration technique [3]. To simulate the motion of the inextensible beam we use an augmented Lagrangian method, whose resulting saddle point problem is solved with an Uzawa-Douglas-Rachford algorithm [2]. Our approach is assessed through various 2D numerical tests. We also show that when the structural displacement is small the results are in good agreement with Arbitrary Lagrangian Eulerian simulations.


An implicit high-order Discontinuous Galerkin solver for hybrid RANS-LES simulations

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Turbulent flows are characterized by a wide range of length and time scales. In fact, while the largest eddies dimension is comparable to that of the body that generated turbulence, the smallest eddies length-scale dramatically decreases with increasing the Reynolds number. For problems of industrial relevance the simulation of all the turbulent scales, i.e., Direct Numerical Simulation (DNS), is nowadays not feasible and some modelling has to be introduced. The governing equations, i.e., Navier–Stokes (NS) equations, can be averaged in time obtaining the Reynolds-Averaged Navier-Stokes (RANS) equations where all the scales are modelled by means of a turbulence model, e.g., $k$–$\omega$. Although the solution of RANS equations is feasible even for high Reynolds numbers, it can be inaccurate in the prediction of some flow features such as massive separation and laminar recirculation bubbles. Large Eddy Simulation (LES) and Detached Eddy Simulation (DES) aim to bridge the gap between no (DNS) and full (RANS) modelling of turbulent scales by solving the large scales of turbulence and modelling the effects of smaller scales by means of subgrid scale (SGS) models. In this work we propose an implicit implementation of the DES-type eXtra-Large Eddy Simulation (X-LES) model of Kok et al.[1] in the Discontinuous Galerkin (DG) solver MIGALE. An accurate space discretization on hybrid type,
highly-stretched and curved, elements is obtained by using hierarchical and orthonormal polynomial basis functions local to each element and defined in the physical space. The time-accurate integration of the fully coupled system of equations is performed by means of linearly implicit Rosenbrock-type Runge–Kutta methods [2], where the exact Jacobian is derived analytically. Assessment and validation of our implementation will be performed by computing external aerodynamics problems that involve massively separated flows, e.g., the flow around a cylinder and a delta wing.


Patient-specific model of the electrical activity in the heart: generation of Purkinje networks driven by clinical measurements

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A key aspect of the heart modeling is the study of electrical activation, that triggers the heart contraction. In particular, the ventricular activation is regulated by the Purkinje fibers (PF), which is the peripheral part of the cardiac conduction system. The PF are isolated from the surrounding muscle except at their endpoints, called Purkinje muscle junctions (PMJ), from which the electrical signal enters the muscle.

The focus of our work is to provide a computational algorithm for the generation of a patient-specific Purkinje network, driven by clinical measures of the electrical activation in the ventricle. The proposed algorithm is based on searching the optimal locations of the PMJ to best fit the measures, computing the activation times in the PF and in the ventricles by solving Eikonal problems.

We tested the accuracy of our method considering five patient-specific geometries with clinical measures acquired during normal and pathological activations. As pathologies, we considered two case of Wolff-Parkinson-White syndrome, one of heart failure and one of Left Bundle Branch Block. The numerical results proved the essential role of a patient-specific Purkinje network, both in modeling the healthy and the pathological activations of the patients under consideration.
Analysis and optimization of the generalized Schwarz method for elliptic problems with application to fluid-structure interaction

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We propose a unified convergence analysis of the generalized Schwarz method applied to a linear elliptic problem for a general interface (flat, cylindrical or spherical) in any dimension. In particular, we provide the exact convergence set of the interface symbols related to the operators involved in the transmission conditions. We also provide a general procedure to obtain estimates of the optimized interface symbols within the constants. Finally, we apply such general results to a fluid-structure interaction model problem, and we assess the effectiveness of the theoretical findings through three-dimensional numerical experiments in the haemodynamic context.
In this talk a mathematical model for the simulation of the mid-ocean ridge will be developed. At the beginning a dimensional analysis is performed on the general conservation laws of continuum mechanics, in order to estimate the magnitude of each term; this is a necessary step which can not be avoided before introducing other hypotheses. The dimensionless model will be then particularized for shallow domains, this kind of approximation will be very useful for the mathematical modeling of large portion of lithosphere. The derived models will be coupled together to define a simplified model of mid-ocean ridge. The analysis will allow also to define suitable boundary conditions for the problem at hand.
Coupling Micro-Scale Dynamics to Collective Behaviors: The Case of Living, hence Complex, Systems

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This communication refers to the modeling of living systems and shows in a number of applications the micro-scale dynamics is transferred to collective behaviors. The first part deals with a methodological approach, while the second part proposes a number of case-studies focusing on biological (multicellular systems) [1],[2],[3], and life sciences.


Optimized partitioned procedures for the Stokes-Darcy coupled problem

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We consider a coupled Stokes-Darcy system for the filtration of an incompressible fluid through a porous medium. The model couples the solution of the Stokes equation in the fluid region, with the solution of the Darcy equation in the porous medium region through the surface separating the two physical domains. Partitioned procedures are modular algorithms commonly used for the solution of coupled multiphysics problems. They involve separate solvers for the different subproblems, that interact in an iterative framework through the exchange of suitable transmission conditions at the multiphysics interface. In the framework of domain decomposition methods, the Robin-type interface conditions introduced in [1] guarantee convergence in the absence of overlap between the different subregions. Following the ideas developed in [2] for Fluid-Structure Interaction problems, we optimize the performance of the corresponding algorithm, both in term of an iterative solver and as a preconditioner for the fully coupled problem [3].


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Fluid-Structure-Interaction in Hemodynamics using Nonlinear, Anisotropic Hyperelastic Wall Models

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We consider the fluid-structure-interaction problem in a blood vessel using a monolithic coupling approach [1], first using a Convective Explicit approach for the fluid. We believe that the prediction of transmural stresses requires the use of sophisticated nonlinear material models for the vessel wall. Fortunately, such models have been developed in the past and their parameters have been adapted to experimental data. Here, we use an anisotropic, polyconvex hyperelastic material model for the structure [2]. The coupled simulations build on the LifeV software library [3] and FEAP [4]. Absorbing boundary conditions on the outflow are imposed to reduce reflections.


A novel implementation of the H-based formulation of the eddy current model

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Eddy current equations are a well-known approximation of Maxwell equations obtained by disregarding the displacement current term (see e.g., [2]). The typical setting for an eddy current problem distinguishes between a conducting region, $\Omega_C$, and the surrounding non-conducting air region, $\Omega_I$. The unknowns of the formulation based on the magnetic field can be reduced to the magnetic field in the conductor $H_C$, the scalar magnetic potential $\Psi_C$ in the insulator and, if the insulator is not simply connected, the loop field $\rho_I$, a curl-free vector field whose line integral on some loops contained in $\Omega_I$ is different from 0. We present a novel implementation of the finite element approximation of the H-based formulation of the eddy current model that uses an alternative procedure for the construction of a basis of the space of loop fields. The proposed method works for general topological configurations and it does not need the determination of “cutting” surfaces (see e.g., [3]). The procedure is based on the explicit knowledge of a maximal set of non bounding cycles on the boundary of the insulator (see [4]), and it uses an explicit formula for expressing the discrete loop fields in terms of linking numbers (see [1]).


Computational models for natural hazards and extreme events simulation
Elliptic problems in arbitrary (possibly infinite) domain and general boundary conditions are center to many applications, like diffusion phenomena, fluid dynamics, charge transport in semiconductors, crystal growth, electromagnetism and many others. In this talk the finite-difference ghost-point method proposed in [1] and its applications are described. The arbitrary domain is defined by a suitable level-set function. The equations are discretized by classical central differences on interior points, while boundary conditions with high order reconstructions are enforced to define the solution at ghost points, which are grid nodes outside the domain with a neighbor inside the domain. The linear system arising from the discretization is solved by a suitable multigrid approach. The numerical method has been successfully employed in several contexts: from fluid-dynamic (incompressible Navier-Stokes and compressible Euler equation) to Elasticity problems (Cauchy-Navier equations). The latter application constitutes the main focus of the present talk, with application to volcanology for computing the displacement caused by pressure sources [2]. In this case the method is extended to treat with infinite domains, by a technique based on a smooth coordinate transformation, which maps an unbounded domain into a unit square.

The overwhelming evidence that climate is changing, including the characteristics of extreme phenomena, poses a challenge to the next generation of numerical weather prediction (NWP) models. The study of the origin and mechanisms determining the location, intensity and frequency of extremes, and how these may change in the future, will indeed require NWP models to be adaptive in order to be able to accurately represent and predict such extremes.

We have introduced an accurate and efficient discretization approach for the shallow water equations on the sphere (extending the technique proposed in [1]), as well as for the non-hydrostatic Euler equations on a vertical slice, that can be effectively applied to all geophysical scale flows [2]. Numerical simulations of classical shallow water and non-hydrostatic benchmarks validate the method and demonstrate its accuracy and efficiency, making it a good candidate for providing the basis of an accurate and efficient adaptive climate and weather prediction system.

We combine a semi-Lagrangian approach with a novel TR-BDF2 based semi-implicit time integrator and with a spatial discretization based on adaptive discontinuous finite elements on hierarchical bases. The resulting method is unconditionally stable and has full second order accuracy in time, thus improving standard off-centered trapezoidal rule discretizations without any major increase of the computational cost nor loss in stability, while allowing the use of time steps up to 50 times larger than those required by stability for explicit methods applied to corresponding DG discretizations.

The method also has arbitrarily high order accuracy in space and can effectively adapt the number of degrees of freedom employed in each element.
in order to balance accuracy and computational cost. The p-adaptivity approach employed does not require remeshing and hence is especially suitable for NWP applications, where a large number of physical quantities has to be reconstructed on the mesh from the available data. Furthermore the p-adaptivity approach can cure the pole problem by reducing the polynomial degree in polar elements, yielding a reduction in the computational cost comparable to that achieved with reduced Gaussian grids.


Numerical-based deterministic methods for earthquake risk analysis in large urban areas

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In this talk we provide an overview of the recent advances on numerical methods for the simulations of earthquake events. We show that numerical-based deterministic methods can be effectively employed to provide realistic earthquake ground shaking maps to be used as the key ingredient to develop earthquake risk scenarios. We present a set of realistic (and physically plausible under the local geological and seismological constraints) extreme earthquake scenarios in key locations worldwide performed with SPEED (http://mox.polimi.it/it/progetti/speed), a new parallel open source code for the simulation of complex wave propagation phenomena jointly developed by the Laboratory for Modeling and Scientific Computing MOX (Department of Mathematics, Politecnico di Milano) and the Engineering Seismology Group (Department of Civil and Environmental Engineering, Politecnico di Milano). From the methodological viewpoint, SPEED is based on a spectral element formulation enhanced by the Discontinuous Galerkin approach for treating non-conforming approximations. After illustrating the SPEED code, we present different case studies and we derive some interesting considerations on the pros and on the limitations of deterministic approaches. This work has been carried out in collaboration with Munich RE (Germany).
Assessing volcanic hazard by using multiphase flow simulations

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Since the 70s volcanologists have successfully described several key features of the dynamics of volcanic eruptions by using mathematical models. First, simple 1D steady-state homogeneous flow models were used to investigate the different eruptive mechanisms of explosive eruptions and to explore the first-order effect of different input parameters. Nowadays, the continuous evolution of those early models has led to the development of a variety of transient, 2D/3D, homogeneous/multiphase flow models of volcanic phenomena implementing state-of-the-art formulations of the underlying physics, new-generation experimental data, as well as high-performance numerical techniques. These numerical models have proved to provide useful insights in the dynamics of explosive eruptions, as well as to represent a valuable tool for the assessment and representation of volcanic hazards. In this talk we will illustrate the application of some multiphase flow models to specific volcanic phenomena (e.g. volcanic jet, pyroclastic density current, ballistic ejecta), to the reconstruction of past events, such as the famous Mt. St. Helens eruption in 1980, as well as to the 2D/3D numerical simulation of possible eruptive scenarios at high-risk explosive volcanoes such as Campi Flegrei and Vesuvius (Italy). We will discuss the challenges and limitations of the different mathematical models as well as of the approach adopted to quantify the volcanic hazard on a probabilistic basis and considering some of the uncertainties affecting the volcanic system.
Lessons learnt from recent earthquakes and the importance of 3D physical modeling in insurance and (re)insurance market

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With the ongoing progress of computing power made available not only by large supercomputer facilities but also by relatively common workstations and desktops, physics-based source-to-site 3D numerical simulations of seismic ground motion will likely become the leading and most reliable tool to construct earthquake ground shaking scenarios. This contribution aims at providing an overview of recent progress on this subject, by taking advantage of the experience gained during a recent research contract between Politecnico di Milano, Italy, and Munich RE, Germany, with the objective to construct ground shaking scenarios from hypothetical earthquakes in large urban areas worldwide. Within this contract, the SPEED (SPectral Elements in Elastodynamics with Discontinuous Galerkin) computer code was developed, based on a spectral element formulation enhanced by the Discontinuous Galerkin approach to treat non-conforming meshes. Different earthquake scenarios will be overviewed, e.g., Emilia-Romagna, Italy 2012 and Christchurch, New Zealand 2011. The comparison with strong motion records allows one to derive some interesting considerations on the pros and present limitations of such approach. Finally, some further development will be presented aiming at drawing the future perspective for this research project.
Variational inequalities, immune systems and local minimizers of functionals
The language of mathematics has been extensively used to describe natural phenomena of the physical sciences in terms of models based on equations. The mathematical language allows logical reasoning over a representation of the physical entities involved in the phenomenon and makes possible to account for the observations made through experimentation.

It is coming nowadays more clear that in order to obtain a unified description of the different mechanisms governing the behavior and causality...
relations among the various parts of a living system, the development of comprehensive computational and mathematical models at different space and time scales are required. This is one of the most formidable challenges of modern biology characterized by the availability of huge amount of high throughput measurements.

In this work, we draw attention to the importance of multi-scale modeling in the framework of studies of biological systems in general and of the immune system in particular.
Duality theory for dynamic vaccination games

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The talk is devoted to an infinite dimensional duality theory finalized to study the existence of a strong duality between a convex optimization problem connected with the management of vaccinations and its Lagrange dual (see [1]). Specifically, the authors show the solvability of a dual problem using as basic tool an hypotheses known as Assumption S (see for details [2], [3], [4]). By using this theory, it is possible to overcome the difficulty of the voidness of the interior of the ordering cone which defines the cone constraints. Moreover, applying the duality theory to the dynamic vaccination game, the Lagrange multipliers associated to the problem are obtained and the behavior of the problem is better understood.


Approximate symmetries of differential equations.

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In many problems of physical interest differential equations contain terms involving "small" parameters. The combined treatment of the theory of Lie groups and perturbation analysis leads to the development of the Theory of approximate symmetries. We consider the above coupled KdV equations

$$u_t + u_{xxx} + 2uu_x + \epsilon [2e_1vu_x + e_2(u_xv + uv_x) + e_3v_{xxx}] = 0$$
$$c_1v_t + v_{xxx} + 2vv_x + c_2v_x + \epsilon c_3[e_1(u_xv + uv_x) + 2e_2uux + e_3u_{xxx}] = 0,$$

(2)

in terms of approximate symmetry reduction approach. The model [1], describes two resonantly interacting normal modes of internal-gravity-wave motion in a shallow stratified liquid. In (2), $u(t,x)$ and $v(t,x)$ represent the displacement from the horizontal of the fluid interfaces, $e_i$ ($i = 1, 2, 3$) and $c_j$ ($j = 1, 2, 3$) are arbitrary constants, while $\epsilon << 1$ is a small parameter. When $\epsilon = 1$ some recent results can be found in [2]. In this paper we perform the approximate symmetry reduction of (2) and approximate solutions are computed by means of the approximate generator of the first order.


2. Ruggieri M. and Speciale M. P. 2013, Similarity Reduction and Closed Form Solutions for a Model Derived from Two Layer Fluids, in Advances in Difference Equations, 355(1), Springer.
This talk is devoted to the study of a general financial equilibrium problem. The problem is modeled by means of an evolutionary variational inequality. In the previous papers [1] and [5], three interesting formulas (deficit formula, balance law, liability formula) were given. These formulas are of great importance for the theory of equilibrium problems evolving in time and they could be of great utility for the management of the world economy. Papers [3] and [4] were the sequel of the previous papers [1] and [5]: we obtained that the solution of the evolutionary inequality is continuous and Lipschitz continuous with respect to time and we illustrated the achieved result through numerical examples. In paper [2] the risk assessment depended on previous equilibria and adaptive constraints were considered. All these
previous papers and results are the basis of this talk in which the utility function includes a memory term and adaptive constraints depending on the expected solution are considered. An existence theorem is proved and significant examples are provided.


A bilevel model of the continuous-time optimal pollution emission price problem

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We consider the problem of the optimal pollution emission price in a continuous-time setting and give a formulation as a bilevel programming problem. In particular, we suppose that control policies are imposed to the end of regulating the pollution emissions of manufacturers in a supply chain. Therefore, the government chooses the optimal price of the pollution emission with consideration to manufacturers’ response to the price. On the other hand, the manufacturers choose the optimal quantities of production to maximize their profits, given the price of pollution emission. Inspired by [1] and [2] and using some new recent results on variational inequalities and infinite dimensional duality, we reformulate the bilevel programming problem into a one level optimization problem. Moreover, the existence of solutions is investigated. Finally, a numerical example is provided.


Inverse variational inequalities and applications to an economic equilibrium problem

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The talk deals with the behavior of control policies whose aim is to regulate the exportation through the adjustments of supply taxes or incentives on the firms (see [1], [2]). Then, we are concerned with a policy-maker optimization problem. This aspect is studied with the help of an inverse evolutionary variational formulation. And, hence, a characterization of the inverse variational inequality with an appropriate evolutionary variational inequality is given. Here the possibility of presence of production and demand excesses is explored. We remark that the definition of equilibrium for the firms is given by using the infinite dimensional duality theory. In order to illustrate theoretical results, we present a numerical example.


Modeling, simulation and optimization of complex systems using Partial Differential Equations
Flow Optimization in Vascular Networks

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The study of mathematical models for vascular networks is very important because of its applications in medicine and pharmacology. The best way to study the arterial system would be to use a 3-D model, but it requires a very high computational power, so we use a 1-D reduced model based on Navier-Stokes equations with appropriate boundary conditions, which still allows to capture the major features under study, such as arterial blood pressure and flow. The simulation is limited by the computational power, so, instead of considering an entire human network, we simulate portions of the network and use inflow and outflow conditions which must realistically mimic the behavior of the network that has been removed from the model. The system is solved numerically using the discontinuos Galerkin scheme and the two-steps method of Adam-Bashfort. The aim is to study the effect of truncation to the flow in the root edge in the case of a fractal network, the effect of adding or subtracting an edge to a given network, the effect of growing a given network in order to obtain the same amount of flow, and optimal control strategies on a network in the event of a blockage or unblockage of an edge or of an entire subtree.


Optimization of the input flow of a supply chain

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The mathematical modeling of supply chains and the development of techniques for simulation and optimization purposes is of great interest in order to reduce bottlenecks, dead times at queues, and so on. Depending on the scale, one can distinguish different modeling approaches. For a recent review see [1].

Here we focus attention on a continuous model for supply chains proposed in [4], according to which a supply chain consists of processors with constant processing rate and a queue in front of each processor. The dynamics of parts on a processor is described by a conservation law, while the evolution of the queue buffer occupancy is given by an ordinary differential equation. We deal with the optimal control problem, where the control is given by the input flow to the supply chain and the cost functional is the sum of the time-integral of queues and quadratic distance from a preassigned desired outflow (see [2, 3]). In particular the controls are the locations of the discontinuities of the input flow of piecewise constant type, while the flux values are fixed. Simulations are performed to show results for the proposed numerical algorithm in some case studies.

2. D’Apice C., Manzo R., Piccoli B. 2012 *Optimal input flows for a PDE-ODE model of supply chains.* Communications in Mathematical Sciences, 10(36), 1226-1240.


A problem of train scheduling on the rail line Verona-Monaco of Bavaria

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As part of a project Industria 2015 called SIFEG (Sistema Integrato Trasporto Merci Ferro Gomma) one of the Promoters, Bertolotti S.p.A, asked to the Master’s candidates Mazzanti and Pungetti to investigate the impact of a freight car of new generation, much faster than those currently in use, about the transport of goods by rail. In collaboration with Trenitalia the railway line on the route Verona-Monaco of Bavaria has been analyzed. The choice of this trait arises from the fact that this route is a real bottleneck for the entry and the exit of goods between Italy and Germany. Applying Operations Research techniques rail traffic was simulated and the impact of the freight wagon of new generation was assessed.


Kernel estimates for Schrödinger type operators with unbounded diffusion and potential terms

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Schrödinger equation gives the quantum description of a particle in an electric field. The ground state of the particle is of relevant importance and it can be related to the heat kernel of the operator. The study of the kernel, furthermore, can be useful for the investigation of spectral properties and pointwise bounds of eigenfunctions of the operator. For this reason we study the kernel of the semigroup generated by a Schrödinger type operator with unbounded coefficient. We consider an operator whose coefficients have a polynomial grow of degree greater than 2 as regards the diffusion part and a lower degree as regards the potential term. We estimate the first eigenvalue of the operator and give heat kernel estimate using the equivalence between the ultracontractivity of the semigroup and a weighted Nash inequality.


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GASVA on Mathematical Modelling in Environmental and Life Sciences
Quasi Steady-State Approximations (QSSAs) in the CME-based stochastic framework

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The Chemical Master Equation (CME) provides an accurate stochastic description of complex biochemical processes in terms of probability distribution of the underlying chemical population. In contrast to deterministic methods, CMEs are therefore considered fruitful stochastic methods for the analysis of biochemical reactions. In the deterministic framework, reactions are usually described by directly expressing the time-evolution of the concentration for each of the involved species, thus leading to having to handle an Ordinary Differential Equation (ODE) system, often of great dimension. To face the analysis of complex processes, the practice to exploit Quasi-Steady State Approximations (QSSAs) has been introduced in literature with the aim of reducing the dimensionality of the system, thus speeding numerical simulations. In this work, we perform a preliminary investigation of the applicability of QSSAs to the stochastic method based on CMEs. To this end, the CME description is applied to the original chemical network, as well as to the standard and total QSS Approximations. The contribution confirms by simulations the effectiveness and superiority of the latter approximation with respect to the former one, also from a stochastic point of view.
Mathematical models for drug delivery are extensively used in bioengineering and provide important contributions to the medical practice, because constitute a powerful predictive tool for a fundamental understanding of biotransport processes. For example, many studies have been carried out to investigate the release properties of a therapeutic drug from a vehicle across the skin, through a transdermal patch.

In order to investigate such a process, a two-phase mathematical model describing the dynamics of a substance between two coupled media of different properties and extents is presented. The first layer is a polymeric platform where the drug is initially contained, and the other one is the skin where the drug is directed to. A set of coupled non-homogeneous partial differential equations describes the diffusion and the reversible binding and unbinding in both layers. Additional flux continuity at the interface and an absorbing condition at the biological medium limit are imposed. An eigenvalue problem is solved and a concentration closed-form solution of the two-phase two-layer model is given in the form of an infinite series expansion.

The typical drug dynamics, the concentration levels, the optimal delivery rate are shown as outcomes of simulations and discussed in some case studies. The results are used to discuss the roles of the diffusion and reaction parameters, to evaluate drug release efficacy and to assess an optimal control strategy in the rational design of advanced delivery systems.
A hybrid mathematical model for self-organizing cells in the zebrafish lateral line primordium

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Lateral line is a sensory system, which is present in fish and amphibians, that is used to detect movement and vibration in the surrounding water, together with other fundamental functions. Zebrafish lateral line represents a model organ which has contributed to a deeper understanding in many fundamental biological issues: interactions between multiple signaling, collective migration during morphogenesis, response of an organ to injury. In this talk [1] we propose a discrete in continuous mathematical model for the morphogenesis of the posterior lateral line system in zebrafishes. Our model follows closely the results obtained in recent biological experiments, [2], [3], [4]. Our description is discrete for the cellular level and continuous for the molecular level. We prove the existence of steady solutions consistent with the formation of particular biological structure, the neuromasts. Dynamical numerical simulations are performed to show the behavior of the model and its qualitative and quantitative accuracy to describe the evolution of this cell aggregate.


Ago-Antagonist Theory in Darwinian Evolution

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In this talk we analyse our proposal on the essential structural aspects of Darwinian Evolution Theory. Using this point of view we apply a mathematical ago-antagonist theory inspired by Y.Cherruault (1998) ideas, which we have extended. In the ago-antagonist model, the phenotype characters measure the individual propensity to perform an innovative $x(t)$ (agonist) or conservative $y(t)$ (antagonist) action with respect to mutations and to speciation process. We have mathematically introduced the conflict concept and we present a model that takes into account the environmental effects by mean of a stochastic multiplicative process. We shortly discuss the properties of the related stochastic differential equations.
Wind-Blown Sand: An Erosion-Transport-Sedimentation-Sliding Model

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Four phenomena are involved in sand movement: erosion, wind transport, sedimentation, sliding. The main reason of erosion of a sand bed is the shear stress exerted by wind on the surface. This is the origin of a phenomenon called saltation, that consists in the raising of sand particles from the soil that then follow a ballistic trajectory influenced by drag and gravity, eventually impacting again on the surface and inducing new particles to detach from the surface. Sand is then transported by the wind and sediment under the action of gravity.

In this talk we will propose a comprehensive multiphase model for sand erosion, transport, sedimentation, and sliding that is then solved in a moving boundary domain. Luckily, the motion of sand grains and the evolution of dune shapes occur on very different time scales which allows the problem to be split and solved in cascade: first determining the flow field, possibly influenced by the presence of grains, then the transport of sand in the domain, and then the evolution of the surface as a consequence of erosion, deposition of sand and redistribution of sand due to the formation of sand avalanches.
Numerical modelling of initial formation in multispecies biofilms

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The work presents a mathematical modelling able to model the attachment phenomena in the initial phase of biofilm growth. In the framework of continuum model, the biofilm growth depends on two main phenomena: biomass growth and substrate diffusion into biofilm [1]. The first is described by a set of nonlinear hyperbolic partial differential equations, the second by a set of semi-linear parabolic partial differential equations. As the physical phenomena, the two sets of equation are mutually connected. The resulting mathematical problem is a free boundary value problem, which is essentially hyperbolic [2,3]. The model has been applied to the biological competition of heterotrophic-autotrophic bacteria in a multi-specie biofilm. The effects of different attachment rates on the biofilm dynamic performances predicting biofilm thickness, volume fractions of bacterial species and substrate concentration trends have been investigated.


A Multidomain Mathematical Model about the Intracellular Transport of Naked DNA Plasmids

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We propose a spazio-temporal model to describe and analyze the intracellular trafficking of naked DNA plasmids. The naked DNA plasmid is extrachromosomal genetic material used in gene therapy to vehiculate therapeutic vectors, that will be transfected into the nucleus. The DNA size of plasmid vectors is between 5 kb and 20 kb, corresponding to 3300-13200 kDa, respectively. The large size of this plasmid not permits the free diffusion in the cytoplasm and the pass across the nuclear envelope. For this reason, we have focused the attention about the role of microtubules in the cytoplasm, and the RAN cycle and the importin through nuclear envelope. Our model is hence a multidomain model: cytoplasm and nucleus in two dimensions, and microtubule in one dimension. Through numerical simulations, we demonstrate and support the experimental data for which the microtubules and the importin are necessary to transport the plasmids into the nucleus. Therefore our results may help to explain how, under certain conditions, the DNA plasmid passes through the cytoplasm and across the nuclear envelope.


Time Scale Separation, Normal Modes and Quasi-Steady State Approximations in Enzyme Kinetics

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The mathematical treatment of enzyme kinetics, based on quasi-steady state approximations, relies on the separation of two different time scales, related to a fast transient phase and a slow phase, where the reactants can be approximately considered in a quasi equilibrium. Several authors have determined sufficient and necessary conditions for the separation of the two time scales in a single reaction, in the framework of the so-called standard quasi-steady state approximation (sQSSA). In the Nineties a new type of quasi-steady state approximation, called total (tQSSA), has been proposed; it is valid in a very large range of parameters and initial conditions, much larger with respect to the standard QSSA. As the classical QSSA, the tQSSA can be interpreted as the leading term of an asymptotic expansion in terms of a suitable parameter. Starting from some papers by Palsson and coauthors in Eighties, we link the tQSSA to the normal modes of the system of non-linear EDOs governing the reactions, aiming at determining a general rule allowing the detection of sufficient conditions guaranteeing the separation of time scales in more general reactions and, consequently, the determination of the appropriate parameters for the corresponding asymptotic expansions.
Numerical Methods and Models for Multiscale Kinetic Equations
High Order Semi-Lagrangian Schemes for the BGK Model

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This talk focuses on the investigation and implementation of high order numerical methods for the solution of the BGK equation in kinetic theory of rarefied gases. This equation governs the evolution of the distribution function of a monatomic gas, and it is a consistent approximation of the Boltzmann equation. The numerical methods are based on a semi-lagrangian formulation [3], that allows us to use larger time steps. The High order in time is obtained in two ways, namely by using Runge-Kutta methods of high order DIRK type, or by using multi-step methods of BDF type. The latter one has the advantage of requiring less interpolation than the DIRK schemes. The High order in space is obtained by using an interpolation technique of WENO type, preventing oscillations. Some applications of these numerical schemes will be presented. One dimensional (in space and velocity) and 3D (in velocity) problems, treated by means of the Chu reduction [1], have been investigated to test the rate of convergence. The methods have been also extended to BGK models for mixtures of inert and reactive gases [1], [2], and reflective and diffusive boundary conditions have been also included, with high order treatment of the boundary.

On the numerical solution of a BGK-type model for chemical reactions,
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Kinetic relaxation models for reacting gas mixtures

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Recent relaxation time-approximation models of BGK type for the kinetic description of chemically reacting gas mixtures are briefly reviewed [1,4]. In spite of their simplicity, their capability in retaining the most significant mathematical and physical properties of the Boltzmann-type kinetic equations made them useful and tractable tools of investigation of chemical reactions in rarefied gas dynamics.

As well known, the main drawback of the BGK approach is an uncorrect prediction of transport coefficients in the continuum limit. To overcome this problem, ellipsoidal (ES) BGK models for inert mixtures have been investigated [2,3]. Moving towards this direction, in this talk we present an ES-BGK model for a slowly reacting binary gas mixture, which is able to correctly reproduce, in the hydrodynamic limit, Fick’s law for diffusion velocities and Newton’s law for the viscous stress.


Derivation of BGK models for gas mixtures

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This paper is devoted to the construction of a BGK operator for gas mixtures. The construction is based as in introduced in some previous works on the introduction of relaxation coefficients and a principle of minimization of the entropy under constraints of moments. These free parameters are compared with the free parameters introduced in the Thermodynamics of Irreversible Processes approach of the Navier-Stokes system. At the end the BGK model is proved to satisfy Fick and Newton laws.
Oxygen transport properties estimation by DSMC-CT simulations

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Abstract. Coupling DSMC simulations with classical trajectories calculations is emerging as a powerful tool to improve predictive capabilities of computational rarefied gas dynamics. The considerable increase of computational effort outlined in the early application of the method [1] can be compensated by running simulations on massively parallel computers. In particular, GPU acceleration has been found quite effective in reducing computing time [2, 3] of DSMC-CT simulations. The aim of the present work is to study rarefied oxygen flows by modeling binary collisions through an accurate potential energy surface, obtained by molecular beams scattering [4]. The accuracy of the method is assessed by calculating molecular oxygen transport properties following three different DSMC-CT simulation methods. In the first one, non-equilibrium zero and one-dimensional rarefied gas dynamic simulations are adopted and the transport properties are computed from the non-equilibrium fluxes of momentum and energy. In the second method, transport properties are obtained from DSMC-CT simulations of spontaneous fluctuation of an equilibrium state [5]. In the third method the collision trajectory calculation has been incorporated with a Monte Carlo integration procedure to evaluate the Taxman’s expressions for the transport properties of polyatomic gases [6]. In Figure 1, preliminary results for the shear viscosity are compared with the experimental results by Lemmond et al. [7]. The three methods provide very close values of shear viscosity, their estimated statistical error not exceeding 3%. The experimental values are slightly underestimated, the percentage deviation being, again, around 3%.
Figure 1: Shear viscosity. Solid line: Experimental results [7], ○ Non-equilibrium simulations, ▲ Spontaneous fluctuations simulations, * Monte Carlo evaluation of Taxman’s collision integrals.


A kinetic BGK model for a multi-component mixture

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We consider a multi component gas mixture without chemical reactions assuming that the number of particles of each species remains constant. We will illustrate the derived model in the case of two species. The two species mixture is modelled by a system of kinetic BGK equations featuring two interaction terms on the right hand side and is motivated by physical considerations. We prove consistency of our model: conservation properties, H-theorem and convergence to a global equilibrium in the shape of a global Maxwell distribution. Thus, we are able to derive the usual macroscopic conservation laws. Finally, by considering a mixture composed of ions and electrons, we derive the macroscopic equations of ideal MHD from our model. This is joint work with Christian Klingenberg (Würzburg University) and Gabriella Puppo (Università Insubria).

Keywords: multi-fluid mixture, kinetic model, BGK approximation, plasma flow
Binary interaction algorithms for the simulation of self-organized systems

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Microscopic models for self-organized systems take into account large numbers of interacting individuals. Numerical resolution of large multi-agent systems implies huge computational costs. Typically for N interacting individuals we have a cost of $O(N^2)$. We tackle the problem numerically by considering approximated binary interaction dynamics described by kinetic equations and simulating such equations by suitable stochastic methods. This approach permits us to compute approximate solutions as functions of a small scaling parameter $\varepsilon$ at a reduced complexity of $O(N_s)$ operations, with $N_s$ the sample size used to reconstruct the kinetic density. Several numerical results show the efficiency of the algorithms proposed and possible extensions.
The mathematics of learning from data
Learning a set by kernel methods

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In this talk I will present a new class of learning algorithms, which allow to estimate the minimal set where the data live on. The main idea is to embed the data, originally described by vectors in $\mathbb{R}^d$ into a bigger Hilbert space $\mathcal{H}$ by means of a feature map in such a way that any closed subset of $\mathbb{R}^d$ is represented by a closed subspace in $\mathcal{H}$. This closed space is hence estimated from the empirical data as the linear span of the first $k$-eigenvectors of the empirical covariance matrix, or a smoother version of it. I will present some general results about the statistical consistency of the algorithm and discuss the role of the zero mean condition. Furthermore, I will comment on the algorithmic implementation and will present a few experiments both on synthetic and real data.
A Unifying Framework for Multi-task Learning

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Multi-task learning is widely acknowledged to be a key approach in reducing the amount of supervision required when distinct but related learning tasks need to be solved simultaneously. The underlying idea is that the system should leverage on task relatedness (structure) to reduce the sample complexity and the amount of necessary labeled data.

In this context, a fundamental question is to develop a framework that allows to incorporate prior information about the tasks, when available, and learn it otherwise. A challenge is to develop the aforementioned framework in such a way as to induce convex learning problems that can be provably solved. To this end, we investigate a regularization approach based on vector-valued reproducing kernels and formulated as a kernel learning problem. We recover most previously proposed methods as special cases.

We introduce a barrier method and notice that, by applying results from optimization theory, the output kernel learning problem can be solved by alternating minimization or inexact block coordinate decent. This can be interpreted as a two step process alternating between supervised and unsupervised learning phases.
A stochastic iteration process with applications to splitting and learning

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This work investigates the properties of stochastic quasi-Fejér monotone sequences in Hilbert spaces and emphasizes their pertinence in the study of the convergence of block-coordinate fixed point methods. The iterative methods under investigation feature random sweeping rules to select the blocks of variables that are activated over the course of the iterations and allow for stochastic errors in the evaluation of the operators. Algorithms using quasi-nonexpansive operators or compositions of nonexpansive averaged operators are constructed. The results are shown to yield novel block-coordinate operator splitting methods for solving structured monotone inclusion and convex minimization problems. In particular, the proposed framework leads to the design of random block-coordinate versions of the Douglas-Rachford and forward-backward algorithms and some of their variants. Applications to learning are discussed.
Dictionary Identification

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In this talk we give an overview over the why and how of dictionary learning. After motivating two flavours of research, sparse coding, from the data processing side and sparse component analysis, from the data analysis side, we focus on the theoretical results for 3 optimisation principles for dictionary identification. We further discuss the local and global efficiency of the corresponding algorithms and draw some conclusions for their use in practice.
Spectral k-Support Norm Regularization

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The k-support norm is a regularizer which has been successfully applied to sparse vector prediction problems. We show that it belongs to a general class of norms which can be formulated as a parameterized infimum over quadratics. We further extend the k-support norm to matrices, and we observe that it is a special case of the matrix cluster norm. Using this formulation we derive an efficient algorithm to compute the proximity operator of both norms. This improves upon the standard algorithm for the k-support norm and allows us to apply proximal gradient methods to the cluster norm. We also describe how to solve regularization problems which employ centered versions of these norms. Finally, we apply the matrix regularizers to different matrix completion and multitask learning datasets. Our results indicate that the spectral k-support norm and the cluster norm give state of the art performance on these problems, significantly outperforming trace norm and elastic net penalties.

In this talk I will present recent advances on the convergence properties of a class of stochastic proximal gradient algorithms for solving minimization problems. These algorithms are easy to implement and suitable for solving high dimensional problems thanks to the low memory requirement of each iteration. Moreover, they are particularly suitable for composite optimization, where a convex objective function is the sum of a smooth and a non-smooth component. I will show that this algorithm can be naturally applied to solve standard online machine learning algorithms and I will focus on convergence in expectation and convergence almost surely of the iterates.

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Mathematical Applications funded by the European Union
This talk concerns the Mathematical Problems arisen within the activity of a Project supported by the PO FESR 2007/2013 subprogram 4.1.1.1 Actions to support the research and experimental development in connection with the production sectors, technological and production districts in areas of potentiality excellence that test high integration between universities, research centers, SMEs and large enterprises. The title of the Project is Mezzo Aereo a controllo remoto per il Rilevamento del TErritorio - MARTE and its objective is the realization of a multirotors system. The multirotor system taken into account is a hexarotor. Assuming the hexacopter as a rigid body, its dynamics is described by the Newton-Euler equations, in which rotations are parameterized in terms of quaternions. Unlike the classical Euler-angle parameterization, they avoid gimbal lock and guarantee more efficiency and stability. A novel PID control, based on quaternions with a linear and simple error, is implemented on an Arduino board with a GPS system to navigate by waypoints and it is maneuvered in manually or automatically way on a selected path or according to its mission.
In the framework of the project SESAMO (Integrated information system for the acquisition, management and sharing of environmental data for decision support), founded European Research Project POR FESR Sicily 2007-2013 – Measure 4.1.1.1, a mathematical model for analyzing water distribution networks, based on the Method Of Characteristic (MOC) was developed. The model is able to simulate the initial filling process, based on the hypotheses that the air pressure inside the network is always equal to the atmospheric pressure and that the water column can not be fragmented, as well as the steady state condition. The network model is integrated with a node demand model based on the node pressure-consumption law, which defines flow drawn from the network for filling the users’s tank. In complex systems characterized by the presence of private tanks and water scarcity conditions, water managers usually apply intermittent distribution, trying to reduce the water volumes supplied to the users and pipe leakages, or use Pressure Reduction Valves (PRV) for controlling pressure in the network. The application of Pumps As Turbines (PATs) appears as an alternative and sustainable solution to either control network pressure as well as to produce energy. In the present paper, the hydrodynamic model, already presented by [1] was further developed introducing a specific dynamic module able to reproduce the PATs behavior. The model was applied to a district of Palermo network (Italy) characterized by intermittent distribution and by inequities among the user in terms of supplied water volumes. The analysis of energy recovery, carried out for a number of different scenarios, shows
that PATs installation can lead to a very attractive economical benefit in term of energy production.

upGraded REnewable ENergy system project

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The aim of the G.RE.EN (upGraded REnewable ENergy system) project is to develop new components which are able to improve the electrical efficiency of photovoltaic and wind power system. The project is granted by PO FESR 2007 - 2013 Asse IV, Obiettivo Operativo 4.1.1 - Linea di Intervento 4.1.1.2. In this project a new bucket configuration for a Darrieus helical wind turbine with three blades is proposed. Numerical analysis was carried out to estimate the performance of the proposed configuration by means of the commercial code ANSYS Fluent. Mathematical problems related to this simulations concern the integration of the Navier-Stokes equations. These equations are solved by using appropriate boundary conditions along all the control volume. The turbulence model adopted is the Transition SST model based on the Menter’s formulation. Parametric studies are performed for a fixed angle of twist ($30^\circ$, $60^\circ$, and $90^\circ$); the results show that for $60^\circ$ angle of twist, the performance of the rotor is improved and evidence a better starting torque. This circumstance is confirmed by static analyses performed on the proposed Darrieus wind turbine configuration.
Within the 7th European Framework a video analysis project has been proposed together with industrial partners aimed at improving safety of workers in chemical plants. The system designed in this project is based on a series of processing stages, based on a state-of-the-art image processing solution specific for each stage.

The overall set of algorithmic tasks can be divided into three main groups, according to their time scheduling, as follows:

Set 1. includes the construction of the geometric models of the cameras, performed in two separated steps. Both procedures are based on the minimization of the error between the computed transformation of calibration points in the scene, and the corresponding image projections. The set of parameters that minimize the error are estimated with the Levenberg-Marquardt optimization algorithm.

The procedure in set 2. is performed continuously in real time, and has the purpose to provide a reliable model of the background. The algorithm used computes a model in the Hue-Saturation-Intensity color space, and adapts automatically the model based on a noise estimation.

The real-time analysis is by itself a sequence of several processing steps. We can again identify two groups of algorithms, depending on their scheduling:

- continuous running analysis;
- multi-camera fusion analysis.
Coherent Structures and Nonlinear Waves
Systems with moving boundaries

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We consider a system of scalar balance laws in one space dimension coupled with a system of ordinary differential equations. The coupling acts through the (moving) boundary condition of the balance laws and the vector fields of the ordinary differential equations. We prove the existence of solutions for such systems passing to the limit in a vanishing viscosity approximation. The results were obtained in collaboration with Professor Mauro Garavello.
Coherent structures and large-scale instabilities in fingering convection

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Fingering convection is a peculiar form of convection with two buoyancy-changing scalars with different diffusivities in which the fluid is unstable even if the overall density decreases upward. Using both direct numerical simulations and analytical theory we show that the fluid self-organizes in blobs that carry the buoyancy anomalies. The appearance of the blobs is responsible for non-Gaussian tails in the probability distribution of the buoyancy fluctuations.

At higher Reynolds number, blobs cluster together and form larger-scale structures which are able to effectively stir the fluid. This phenomenon leads to the formation of step-like profiles in the horizontal averages of density and of the two scalars. The formation of steps has often been attributed vaguely to some form negative diffusion process, due to the fact that fingering convection carries density up-gradient. A mathematical model that describes the dynamics of the horizontally-averaged scalar fields and the staircase-forming instabilities elucidates the proposed process of staircase formation, while avoiding the ill-posedness of naive negative-diffusion approaches.


Oscillating Turing patterns and spiral wave behavior in a mathematical model for alloy electrodeposition

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Metal growth by an electrochemically controlled process is known to exhibit peculiar instabilities that have a crucial impact on the quality of the material and on its functional properties. We consider a novel mathematical model for alloy electrodeposition which accounts for the coupling between surface morphology and surface composition as a means for understanding the formation of morphological patterns found in electroplating. We study Turing and Hopf instabilities and analyse the codimension-2 Turing-Hopf bifurcation. As a result, we detect and characterize classical Turing patterns as well as oscillating Turing patterns. In the Hopf region, we prove the existence of spiral wave behavior and observe the emergence of complex spatio-temporal behavior via spirals break up. We investigate the model spatio-temporal dynamics from both the analytical and numerical points of view obtaining classes of morphogenetic scenarios in good qualitative accordance with experiments.


Second-grade nematic fluids and nematoacoustics

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There is plenty of experimental evidence that the propagation of an ultrasonic wave in a nematic liquid crystal affects the director \( \mathbf{n} \), which represents the average molecular orientation, thus producing detectable optical effects. There have been several attempts to explain these observations on the basis of a coherent variational theory. We present here a general theory for nematoacoustics that incorporates flow effects. Applications of the proposed theory are also provided. Firstly, an explicit application to a simple computable case is given in order to estimate phenomenological parameters involved in the theory and by using available experimental data. In particular, propagation of plane waves is considered via linearization of the governing equations stemming from the general theory. Secondly, we introduce the equations that have been derived from the basic theory and that govern the nematoacoustic streaming in liquid crystals. Thirdly, travelling wave solutions are also shown in a simple one-dimensional nonlinear reduced model. Finally, if time permits, we sketch the solution for the so-called Freedericks transition by considering the coupling with an electric field.

**Keywords:** wave propagation, nematic liquid crystals, acoustics, variational theory, Freedericks transition

**References:**


The heat transfer problem is one of the simplest case of non-equilibrium thermodynamics, but in spite of its simplicity, several questions are still open both from the theoretical and from the experimental point of view. In particular, very few experimental data are available in the literature.

In this talk we will consider a gas or a gas mixture confined in a bounded domain under the assumption that the walls are kept at different temperatures. Referring to the Extended Thermodynamics [1] approach we will study the non-linear effects, the role of the domain geometry and that of the gas rarefaction, the differences due to the materials (monoatomic or polyatomic gases, gas mixtures) [2-4], the effects of a non inertial frame or of a rotating wall [5]. The results will be compared with experimental data or with Monte Carlo simulations, when available. The features of the solution behaviour will be analysed and the differences between Classical and Extended Thermodynamics predictions will be investigated.


Signal and image processing techniques, and applications
We collect some results concerning electrical conduction problems in biological tissues. Indeed, it is well known that electric potentials can be used in diagnostic devices to investigate the properties of biological tissues. Besides the well-known diagnostic techniques such as magnetic resonance, X-rays and so on, it plays an important role a more recent, cheap and noninvasive technique known as electric impedance tomography (EIT). Such a technique is essentially based on the possibility of determining the physiological properties of a living body by means of the knowledge of its electrical behavior ([5], [6]).

The models we present here are described by means of a finely mixed periodic medium, with a very small characteristic length, made by two different conductive regions (the intracellular and extracellular spaces), separated by an interface (the cell membrane), which exhibits both a capacitive and a conductive behavior. Due to the biochemical structure of the cell membrane, its conductive properties can perform a linear or a nonlinear behavior. We will discuss these two different situations, producing in each case a “macroscopic” or “homogenized” model, obtained letting the spatial period of the medium go to zero ([1], [3]). The asymptotic behavior of the macroscopic potential for large times is investigated, too ([2], [4]).


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Image Contrast Enhancement by means of Fuzzy Techniques

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Within the image processing, the contrast enhancement represents one of the most important procedures because of the rst step of perceptible enhancement of the quality of an image. Technically, the procedures of contrast enhancement can be divided into two main categories. The rst, of indirect type, modyes the histogram of the image through the assignation of new values of levels of grey in each pixel. Indirect approaches, already consolidated in literature, are the histogram specication and/or equalization [1], [2]. On the contrary, the procedures of direct type act on the formulation of a criterion of measurement of the contrast: the enhancement of the quality of the image occurs through the improving of such measure [3], [4]. The images, however, are not free from uncertainties and/or imprecision, so it appears evident the necessity to formulate algorithms of contrast enhancement based on fuzzy criteria. In such work, the author presents a new approach for the contrast enhancement based on fuzzy formulations of statistical-geometrical type exploiting synergies between statistics of growing order, entropy evaluations and fuzzy similarities inside unitary hyper-cubes. The features, extracted directly from the image under examination by means of a procedure with a reduced computational complexity, let the procedure be automatic characterizing its adapteness. The results obtained are wholly comparable both in qualitative and quantitative form with those got with consolidated techniques and encourage further studies in depth.


Topology preservation of radial basis functions for image registration

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Image registration consists mainly in finding a suitable transformation between two images, called source and target images, taken either at different times or from different sensors or viewpoints. The scope is to determine a transformation such that the transformed version of the source image is similar to the target one. There is a large number of applications demanding image registration, for an overview see e.g. [2]. In this talk we focus on landmark-based image registration, in particular on the topology preservation of radial basis functions (RBFs) transformations. Many RBFs are used to model deformations. In [1] the performances of Gneiting’s and Wu’s functions are compared with the ones of other well known schemes in image registration, as thin plate spline and Wendland’s functions. Several numerical experiments and real-life cases with medical images show differences in accuracy and smoothness of the considered interpolation methods, which can be explained taking into account their topology preservation properties. Here we analyze analytically and experimentally the topology preservation performances of Gneiting’s and Matern functions, comparing results with the ones obtained in [3], where Wendland’s and Wu’s functions are considered.


A Semi-Analytic Bayesian Approach for Multiple Static Dipoles Estimation from a Time Series of MEG Data

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Magnetoencephalography is a non-invasive functional neuroimaging technique used to reconstruct neuronal currents from the weak magnetic field recorded.

In a dipolar model framework neuronal currents are approximated as point-like sources, difficult to estimate because of the ill-posedness of the inverse problem and because the number of active regions is typically unknown and is usually estimated heuristically. Extending the work in [1] we present a novel Bayesian computational method that exploits the linear dependence of the data over the dipole moment and is able to estimate the number of active dipoles, their location and strength, from both single topographies and full MEG time-series under the assumption that the number of sources and their position are fixed over time.

In particular we show that assuming a Gaussian distribution for the dipole moment and for the noise model we can approximate the posterior distribution for the number of dipoles and their location through Sequential Monte Carlo sampler and then we can compute analytically the conditional posterior distribution for the dipole moment.

We test our method with both real and simulated data which show that it produces good approximations with both correlated and uncorrelated sources.

Nowadays, the brain activity can be investigated non-invasively by means of electromagnetic techniques, namely electroencephalography (EEG) and magnetoencephalography (MEG). Such techniques require a typical inverse problem to be solved. Therefore, an accurate and fast forward solver has to be employed. As an alternative to the Boundary Element Method (BEM), which involves both complex meshing algorithms in the pre-processing stage and costly numerical integration routines, we propose the application of a truly meshfree solver for the numerical solution of the M/EEG forward problem, i.e., a set of coupled boundary value problems for the 3D Laplacian operator. The proposed method is based on the Method of Fundamental Solutions (MFS) and the Method of Particular Solutions (MPS), so it has potential for spectral accuracy and it is integration-free. Flexibility and remarkable simplifications in the pre-processing stage are also reached. Numerical experiments on spherical head geometries, for which analytical or
semi-analytical solution of the potential problem are known, show the potentiality of the proposed method when it is compared to the state-of-the-art BEM by considering both numerical accuracy and computational cost. Results of experiments conducted on real head geometries are also shown.


Here different Bäcklund Charts are considered both in the case of Commutative Equation Hierarchies as well as in the case of their Non-Commutative analogues. The aim is to point out differences and analogies\textsuperscript{[1]}. Specifically, the case of the Cole-Hopf link between Burgers and Heat Equations \textsuperscript{[2, 3]} and its extension to the corresponding Hierarchies are considered \textsuperscript{[4]}. Furthermore, links connecting third order nonlinear evolution equations, such as KdV, mKdV are analyzed, again, in both the commutative \textsuperscript{[5]} and non-commutative case \textsuperscript{[6]}. Notably, the latter give rise to a wider variety of equations. Correspondingly, various different hierarchies of non-commutative equations are generated while, in the commutative case, there was only one hierarchy. Furthermore, the related recursion operators are considered pointing out their peculiar properties in the non-commutative case. These properties, already directly proved in previous works, can be, now, verified on use of a computer algebra program ad hoc devised \textsuperscript{[7]} to verify the algebraic requirements which characterize recursion operators.


An anisotropic multiple multiresolution analysis for image data processing

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The concept of multiple multiresolution analysis in $L^2(\mathbb{R}^2)$ has recently been introduced [2] as an extension of the classical wavelet setting. In such an approach, each step of the filterbank implementation can be controlled by different scaling matrices and filters, chosen from a finite dictionary, allowing for a directionally adapted processing of the data, so that, for example, singularities along lines can be handled. In this talk, we restrict to the bidimensional case and present a strategy for multiple filterbank construction based on expanding matrices presenting anisotropic properties and very small determinant. This implies a considerable reduction in terms of computational efforts for processing image data, compared with the well-known discrete shearlet transform [1]. After discussing about the filter construction strategy and the slope resolution property of our scheme, we will present a few examples of applications.


A BeamFormer for source localization in ElectroCOrticoGraphy

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ElectroCOrticoGraphy (ECoG) is a neuroimaging technique measuring the electrical potential distribution produced by the neural currents by means of a sensors grid implanted on brain surface. Recording from the inside the brain electrical activity provides a signal with high signal-to-noise ratio, which can be used to validate other non-invasive neurophysiological techniques like magneto- and electroencephalography [1]. In the last few years, some papers on methods to solve the ECoG inverse problem [2] of reconstructing the spatio-temporal distribution of the neural currents responsible of the recorded signal are presented in literature.

This study addresses the ECoG source modelling developing a beamformer method. First, the lead-field matrix, mapping the neural currents onto the sensors space, is created by using a new function provided by the OpenMEEG software [3]. Then, a systematic study of the numerical stability associated to the ECoG inverse problem is performed by analyzing the condition number of the lead-field matrix. Finally, the source localization is realized by applying a spatial filter to both synthetic data and experimental measurements recorded under visual stimulation.

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On the problem of recovering non regular surfaces from gridded data

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In this talk we discuss the problem of recovering a non regular surface from a set of gridded data. By non regular surface, we mean that the function underlying the data or its gradient are discontinuous along a curve: fault in the first case and gradient fault in the second.

This topic is of great interest in many applied problems, in fact surfaces with discontinuity curves appears in many scientific applications including signal and image processing, geology, geophysics, economics, medicine. For instance, in the analysis of medical images as the magnetic resonance (MRI) the fault lines may indicate the presence of some pathology. In many problems of geophysical interest, one has to deal with data that exhibit faults and also gradient faults. This occurs when describing the topography of seafloor surfaces, mountains with drainage patterns and in general the shape of geological entities. In any case, discretely defined surfaces that exhibit such features can not correctly recovered without the knowledge of the position of the discontinuity curves and the type of discontinuity. The typical problem that occurs is over-smoothing near gradient faults and Gibb’s phenomenon near the faults. In general the solution of the problem consists of two steps. First we need to detect the discontinuity curve, to know the kind of discontinuity and to approximate it faithfully. Secondly, with these information we can recover the surface.

We assume that the discontinuity curve is known, and we propose an interpolatory strategy which provides a satisfactory and effective solution to the problem. The method is based on the Generalized Whittle–Matérn kernels. Starting from these generalized kernels we construct an interpolatory subdivision scheme based on the lagrangian function associated with this new kernels.
Magnetic Tomography by Random Spatial Sampling

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The Magnetic Tomography (MT) is an imaging technique that aims at reconstructing an unknown electric current distribution flowing within a volume conductor from the measurements of its magnetic field in the outer space. Among the other imaging techniques, MT has the advantage to be noninvasive and to have a high temporal resolution. For these reasons MT has applications in several fields, from geophysics to archeology, from nondestructive analysis of structures to medical tomography [1].

MT devices do not give immediately an image of the electric current that flows in the conductor under study. Actually, to reconstruct the unknown current distribution from the magnetic data an highly ill-posed and ill-conditioned inverse problem has to be solved. We propose to solve the MT inverse problem by an inversion method based on the random sampling of the source space. The main advantage of the method is the dimensionality reduction that makes the method fast and the storage requirements very low. Moreover, the method can be easily applied to conductors of any shape.

Some numerical tests showing the performances of the method on both synthetic and real data will be shown.

Design of a portable (CW) fNIRS embedded system

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This paper deals with the design of a portable Continuous Wave (CW) functional Near InfraRed Spectroscopy (fNIRS) system for monitoring haemodynamic signals during brain activity. It can only provide oxygenated and deoxygenated haemoglobin changes [2]. The prototype is based on a scalable architecture composed by 8 modular probes, built on flexible stand, each one containing 4 bi-color LEDs, 16 photo-detectors and a temperature sensor. Hardware originality is obtained by adopting Silicon PhotoMultiplier (SiPM) optical sensors which could also increase the spatial resolution of the fNIRS system [1]. The hardware structure allows to easily configure, thanks to an ARM microcontroller, several parameters: the switching time and the optical power radiated by each LED; the acquisition and the working voltage of each SiPM. Moreover, it is possible to choose the portion of cerebral cortex to be analysed, by choosing the LED-SiPM couples that will be involved in the measurement [3]. Furthermore, in order to display the haemoglobin changes induced by brain activity (or possible diseases), raw data are elaborated by the modified Beer-Lambert’s law and then they are filtered through a 300 mHz low-pass filter so to reject the unwanted cardiac pulses [4]. Several preliminary functional tests were successfully carried out, thus achieving very encouraging results.


Wavelet packet as diagnostic tool: an EEG study

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The aim of the study is to investigate a feature extraction method of an Electroencephalogram (EEG) by means of wavelet packet for discrimination of two cognitive stages: Alzheimer disease (AD) and Mild Cognitive Impairment (MCI) [1]. MCI is a term used to describe subjects who experience temporary lack of memory, but in a less severe manner if compared to AD, clinically characterized by serious impairments of memory and other cognitive functions. Fifty-five subjects (n=17 AD, n=19 MCI, n=19 Control), age range 72.0 ± 9.0 years have been enrolled for this study. EEG signals were recorded from 19 electrodes in resting state condition. The idea is to employ wavelet packet to extract two features (mean and energy coefficients) for different frequency bands ([5 – 20] Hz) and 8 most significative channels for each group. Firstly, original EEG signals are sub-sampled and filtered. Then, signals are decomposed to the sixth level of wavelet packet transform. Finally, qualitative (Cluster Analysis) and quantitative (Mixed Effect General Linear Model) analysis are performed to different subbands focusing on extracted features. The results demonstrate that coefficients energy better discriminate cognitive impairment compared to coefficients mean, leading to a disease marker potentially able to monitor diagnosis ongoing status.

Bäcklund Charts: commutative versus non-commutative Equation Hierarchies

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Here different Bäcklund Charts are considered both in the case of Commutative Equation Hierarchies as well as in the case of their Non-Commutative analogues. The aim is to point out differences and analogies\[1\]. Specifically, the case of the Cole-Hopf link between Burgers and Heat Equations \[2, 3\] and its extension to the corresponding Hierarchies are considered \[4\]. Furthermore, links connecting third order nonlinear evolution equations, such as KdV, mKdV are analyzed, again, in both the commutative \[5\] and non-commutative case \[6\]. Notably, the latter give rise to a wider variety of equations. Correspondingly, various different hierarchies of non-commutative equations are generated while, in the commutative case, there was only one hierarchy. Furthermore, the related recursion operators are considered pointing out their peculiar properties in the non-commutative case. These properties, already directly proved in previous works, can be, now, verified on use of a computer algebra program ad hoc devised \[7\] to verify the algebraic requirements which characterize recursion operators.


In this talk, we present the theory of multivariate sampling Kantorovich operators and their applications to image processing [1, 4, 5]. In particular, applications to thermographic images for civil engineering and to medical images will be shown, see e.g., [3]. The above discrete operators are defined by:

\[ (S_w f)(x) = \sum_{k \in \mathbb{Z}^n} \chi(w x - t_k) \left[ \frac{w^n}{A_k} \int_{R^w_k} f(u) \, du \right] \quad (x \in \mathbb{R}^n, \ w > 0), \quad (I) \]

where \( \chi : \mathbb{R}^n \to \mathbb{R} \) is a kernel function satisfying the usual assumptions of the approximate identities, \( t_k = (t_{k_1}, \ldots, t_{k_n}) \), \( (t_{k_i})_{k_i \in \mathbb{Z}}, \ i = 1, 2, \ldots, n \), are strictly increasing sequences of real numbers, \( R^w_k := \left[ \frac{t_{k_1}}{w}, \frac{t_{k_1}+1}{w} \right] \times \left[ \frac{t_{k_2}}{w}, \frac{t_{k_2}+1}{w} \right] \times \ldots \times \left[ \frac{t_{k_n}}{w}, \frac{t_{k_n}+1}{w} \right] \), and \( A_k := \Delta_{k_1} \cdot \Delta_{k_2} \cdot \ldots \cdot \Delta_{k_n} \) with \( \Delta_{k_i} := t_{k_i+1} - t_{k_i} \), \( i = 1, 2, \ldots, n \). The function \( f : \mathbb{R}^n \to \mathbb{R} \) is a locally integrable function such that the above series is convergent for every \( x \in \mathbb{R}^n \). First, the theoretical approximation results involving bounded continuous and uniformly continuous functions are discussed, together with a modular approximation theorem for functions belonging to Orlicz spaces (see e.g., [2]). The algorithm for image reconstruction based on sampling Kantorovich operators is described and several numerical examples and applications are shown.
Recent advances on the theory and applications of Semi-Lagrangian methods
A Semi-Lagrangian scheme for a degenerate second order Mean Field Game system

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We present a fully discrete Semi-Lagrangian approximation of a second order Mean Field Game system, which can be degenerate. We prove that the resulting scheme is well posed and, if the state dimension is equal to one, we prove a convergence result. Some numerical simulations are provided, evidencing the convergence and the difference between the numerical results for the degenerate and non-degenerate cases.


Semi-Lagrangian methods have traditionally been developed in the framework of hyperbolic equations, but several extensions of the SL approach to diffusion and advection–diffusion problems have been proposed recently, see e.g. [1],[2]. These extensions are mostly based on probabilistic arguments and share the common feature of treating second-order operators in trace form, which makes them unsuitable for classical formulations of turbulent diffusion employed in computational fluid dynamics and for mass conservative models. We propose here some basic ideas for treating second-order operators in divergence form. A general framework for constructing consistent schemes in one space dimension is presented, and a specific case of nonconservative discretization is discussed in detail and analysed. Finally, an extension to problems in an arbitrary number of dimensions is proposed. Although the resulting discretization approach is only of first order in time, numerical results in a number of test cases highlight the advantages of these methods for applications to computational fluid dynamics and their superiority over to more standard low order time discretization approaches.


2 Falcone, M. and Ferretti, R. 2013 Semi-Lagrangian Approximation Schemes for Linear and Hamilton-Jacobi Equations. SIAM
Semi-Lagrangian approximation schemes for non-Lambertian Shape-from-Shading models

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Shape-from-Shading (SfS) is a classical problem in computer vision. It uses the brightness variation in a single image to compute the three dimensional shape of a surface and leads to a nonlinear partial differential equation (PDE) of the first order \cite{3,2}. Two tasks have to be accomplished in solving the SfS problem. The first is to formulate an imaging model that describes the relation between the surface shape and the image brightness. This relation should consider the three components of the problem which are the camera, the light source and the surface reflectance. After establishing the imaging model, a numerical algorithm has to be developed to reconstruct the shape from the given image. In this talk we focus our attention on this last numerical issue, fixing orthographic projection of the scene, one light source located at infinity and choosing three reflectance models (the classical Lambertian model and two of non-Lambertian type \cite{1}, namely the diffuse Oren–Nayar model \cite{4} and the specular Phong model \cite{5}). We construct a semi-Lagrangian scheme corresponding to each PDEs coming out, analyzing the properties of the operators involved. Then, a comparison of their performance will be given in terms of some error indicators on series of benchmarks images.
Bibliography


Fast Semi-Lagrangian Schemes for Hamilton-Jacobi-Bellman Equations

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Hamilton-Jacobi-Bellman (HJB) equations arise in several contexts, including optimal control problems for nonlinear ordinary differential equations with state/control constraints. Unfortunately, when the state dimension is larger than three, both single-pass and iterative numerical methods for HJB equations are hardly usable since they require a huge computational effort and memory allocation.

In this talk we investigate the possibility to use the Fast Iterative Method (FIM) [3] for solving general HJB equations and we compare the results with a new accelerated version of the Fast Sweeping Method (FSM) [4]. We find that FIM can be indeed used to solve HJB equations with no relevant modifications with respect to the original algorithm proposed for the eikonal equation, and that it overcomes FSM in many cases.

Observing the evolution of the active list of FIM, we recover another numerical validation of the arguments recently discussed in [2] about the impossibility of creating local single-pass methods for HJB equations.


Experiments on adaptive semi-Lagrangian advection in a DG framework

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Advection experiments are shown in the context of a high-order Discontinuous Galerkin semi-Lagrangian technique, with a focus on atmospheric applications.

Discontinuous Galerkin methods are high order schemes that allow high flexibility but their combination with standard explicit time integrators is characterized by strong stability restrictions, a significant limitation if numerical weather prediction or even climate applications are envisaged.

The combination of DG methods with the semi-Lagrangian technique provides an unconditionally stable discretization for advection, which is relevant for such geophysical applications [1].

We present some numerical experiments on advection both in Cartesian and spherical geometry, where the efficiency of the semi-Lagrangian DG discretization is improved through the introduction of a p-adaptivity strategy to effectively adapt the number of degrees of freedom employed in each element, taking advantage of the locality typical of DG and of the use of hierarchical bases [2], [3], [4].


High order schemes for nonlinear evolutionary Partial Differential Equations
Several systems of evolutionary partial differential equations may contain stiff terms, which require an implicit treatment. Typical examples are hyperbolic systems with stiff hyperbolic or parabolic relaxation and kinetic equations in regimes close to fluid dynamic limit. In many cases, the stiff terms are clearly identified. For example, in hyperbolic systems with hyperbolic relaxation, the hyperbolic term is usually non stiff, while the relaxation term is stiff. A natural way to treat such systems is to adopt implicit-explicit schemes, in which the relaxation is treated by an implicit scheme, while the hyperbolic part is treated explicitly. In several cases, however, such a distinction is not so clear. For example, in the case of hyperbolic systems with diffusive relaxation, a standard approach would lead to schemes, which in the stiff limit suffer from classical parabolic CFL restriction. Such systems can be treated by a penalization method, consisting in adding and subtracting the same term, so that the system appears as the limit relaxed system plus a small perturbation. There are cases, however, in which stiff terms are not just additive, and the penalization method is not particularly effective, since the limit system itself is not easily solvable by standard techniques. For many such systems, we present a new approach, which includes partitioned and additive approach. It consists in identifying the linearly stiff dependence of the system on the unknown variable. Only this linear dependence will be treated implicitly, while the rest of the system is treated explicitly. This approach generalizes classical IMEX schemes based on additive or partitioned Runge-Kutta methods, and allows the construction of high order linearly implicit schemes, which are much simpler to use than fully implicit ones. Several examples will be presented.
In this talk we compare and study several numerical approaches for time integration in order to obtain all-speed, asymptotic preserving and unconditionally stable numerical schemes for hyperbolic systems containing sti relaxation source terms [1, 2, 3, 4]. Such models arise in many physical problems, as in the modelling of multiphase flows involving phase transitions, kinetic-type phenomena, semiconductor devices, and biological systems. As an example, we can mention isentropic Euler equations, Euler equations with linear friction, radiative transfert models, Euler-Poisson systems. The presence of the sti relaxation term allows to describe distinct physical time-scales terms, which can exhibit different behaviours, from hyperbolic to diffusive regime. The study and the numerical approximation of these models is particularly challenging, as several aspects have to be handled. We present several numerical experiments and comparisons together with some preliminary theoretical results and considerations.


Implicit-Explicit Runge-Kutta schemes for optimal control problems and applications to hyperbolic system with relaxation

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Implicit-explicit (IMEX) Runge-Kutta methods play a major role in the numerical treatment of differential systems governed by stiff and non-stiff terms. In this talk we discuss order conditions and symplecticity properties of a class of IMEX Runge-Kutta methods in the context of optimal control problems. Using suitable transformations of the adjoint equation, order conditions up to order three are proven as well as the relation between adjoint schemes obtained through different transformations is investigated. Conditions for the IMEX Runge-Kutta methods to be symplectic are also derived. We finally present some applications of the developed schemes to hyperbolic systems of partial differential equations with relaxation.

Joint work with L. Pareschi (Università di Ferrara), C. Jörres, M. Herty and S. Steffensen (RTWH Aachen).
High order exponential schemes for nonlinear Fokker-Planck equations

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In this talk we present some recent results on the construction of high-order exponential schemes for nonlinear Fokker-Planck equations. The schemes are able to avoid the parabolic stiffness and to achieve the asymptotic-preserving property at the cost of an explicit method. The main advantage compared to IMEX methods is the possibility to achieve very high order accuracy without introducing additional order conditions. Applications to the Landau equation of plasma physics are presented.
Mathematical Problems from micro and nano-electronics industry
Analytical and numerical characterization of the spin-wave properties emitted in a spintronic nano-waveguide

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Spin-wave dynamics induced by the combined action of magnetic fields and electric currents have been receiving a great deal of attention from theoreticians and experimentalists for the intriguing properties exhibited by the nano-sized devices where such magnetization dynamics are observed [2] as well as for their industrial applications [3]. In this work we consider a ferromagnetic heterostructure in the form of a one-dimensional waveguide. In this geometry, a localized excitation via an electric current favors the emission of spin-waves which are conveyed along the axis of the guide. The functional dependence of the main characteristic wave parameters (threshold current, frequency, wavenumber and decay length) is analyzed as a function of the size of the nanocontact area through which the electric current is injected. From the analytical viewpoint, such a goal has required to solve the Landau-Lifshitz-Gilbert-Slonczewski equation [4] together with boundary and matching conditions associated to the waveguide geometry [1]. Owing to the complexity of the resulting transcendent system, particular solutions have been obtained in the cases of elongated and contracted nanocontacts. These results have been successfully compared with those arising from numerical integration of the abovementioned system and with micromagnetic simulations based on finite-differences methods.


Particle Laden Turbulent Shear Layers
On the importance of modeling the fluid acceleration term in a particle laden, compressible turbulent boundary layer

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Numerical computations of turbulent flows customary just use the most obvious term $\frac{d u_{p,i}}{d t} = -1/\tau_p (u_{p,i} - u_{f,i})$ of the Maxey Riley equation to model the fluid forces acting upon a particle. We found the fluid acceleration term $\rho_f \frac{D u_{f,i}}{D t}$ is equally important or even dominant in shock particle interaction [1,2]. Recently was reported that the basset history force is important in isotropic turbulence and in sedimentation processes in two dimensional convection flows [3]. It turns out that both terms are customarily neglected either on ground of mere convenience or difficulties in computing them. Here we present a study which aims at pointing out the importance of the fluid acceleration term in a turbulent boundary layer at $Re_{\delta, in} = 4700$ and $Ma = 0.8$ on a flat plate. The Reynolds number is based on the inlet boundary layer thickness.

Our particle to fluid density ratio $\rho_p/\rho_f$ is around 2000, the Stokes number based on the inlet conditions is $St \approx 0.2$ and we have a volume fraction of order $\mathcal{O}(10^{-4})$.

The turbulent compressible boundary layer is simulated with a characteristic-type formulation of [4], high order compact finite difference schemes and a Runge-Kutta of fourth order for time integration.


Exact regularized point particle method for particle-laden flows in the two-way coupling regime: application to turbulent free shear flows

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Abstract: In this paper we present a new methodology which captures the momentum exchange between a carrier turbulent flow and hundreds of small inertial particles. The velocity disturbance produced by the disperse phase is described analytically in terms of an exact regularized unsteady Stokes solution. Results for actual turbulent flows laden with sub-Kolmogorov particles are discussed and the turbulence modulation is addressed in two typical free shear flow configurations, e.g. a homogeneous shear flow and a round jet.

The effect of turbulent transport on particle dynamics has been extensively studied in many flow configurations. Much less is known about the effect of the disperse phase on the carrier flow demanding for a renewed effort in this direction, see e.g. [1]. In the so-called two-way coupling regime the particles volume fraction is still small to neglect particle/particle collisions and hydrodynamic interactions but the mass loading on the fluid might result of order one due to large density ratios. In such conditions the momentum exchange between the two phases is not negligible and must be properly accounted for.

Modeling the back reaction in numerical simulations is an issue. The local distortion of the carrier flow due to the disperse phase can be captured only resolving the boundary of each particle on the computational grid. In the so-called resolved particle simulations several approaches have been proposed to enforce the non slip boundary conditions on the particle boundary, see e.g. [2]. Alternative approaches are possible once recognized that the flow close to a small particle can be locally approximated by a Stokes Flow, [6, 4].

The approaches discussed so far, are feasible only for a relatively small number of large particles i.e. of particles whose diameter $d_p$ is larger than the smallest fluid scale, i.e. the Kolmogorov scale $\eta$. However in many
applications hundred thousands of small particles are carried by the flow and such methods can not be pursued. Our new approach is intended to describe the inter-phase momentum coupling for particles whose size ranges from sub-Kolmogorov dimensions up to a few Kolmogorov scales where physically sound and computational efficient approaches are still lacking.

The inter-phase momentum coupling is achieved in terms of an exact solution of the local unsteady Stokes flow around each particle. In a nutshell, it is possible to evaluate in a closed analytical form the vorticity that each particle generate along its trajectory. Due to viscous diffusion the disturbance vorticity reaches length-scales comparable to the smallest hydrodynamical scales where the disturbance field can be transfered and represented on the computational grid where the Navier-Stokes equations of the carrier fluid are solved. The momentum coupling between the two phases is based on this physical mechanisms and does not require any “ad hoc” numerical artifacts. In fact, due to the small value of the particle Reynolds number, the distur-
bance flow produced particle is well described by the incompressible Stokes equations, \( \partial_t \mathbf{v} - \nu \nabla^2 \mathbf{v} + \nabla p = \mathbf{F} \), where \( \mathbf{F}(\mathbf{x}, t) = -D(t) \delta [\mathbf{x} - \mathbf{x}_p(t)] \) is the (singular) force that the particle exerts back on the fluid. \( D(t) \) is the hydro-
dynamic force, \( \delta(\mathbf{x}) \) is the Dirac delta function and \( \mathbf{x}_p(t) \) the actual position of the \( p^{th} \) particle. To regularize the effects of the singular back-reaction on the fluid we exploit the localization operated by the intrinsic diffusion of the vorticity field generated by the particle motion \( \zeta = \nabla \times \mathbf{v} \),

\[
\frac{\partial \zeta}{\partial t} - \nu \nabla^2 \zeta = \nabla \times \mathbf{F} = D(t) \times \nabla \delta [\mathbf{x} - \mathbf{x}_p(t)]. \tag{3}
\]

The regularization procedure is based on a temporal cut-off \( \epsilon_R \) such that the vorticity is additively split into a regular and a singular component, \( \zeta(\mathbf{x}, t) = \zeta_R(\mathbf{x}, t, \epsilon) + \zeta_S(\mathbf{x}, t, \epsilon) \). It is easy to derive the differential equation satisfied by \( \zeta_R(\mathbf{x}, t) \) namely

\[
\frac{\partial \zeta_R}{\partial t} - \nu \nabla^2 \zeta_R = -\nabla \times D(t - \epsilon_R) g [\mathbf{x} - \mathbf{x}_p(t - \epsilon_R), \epsilon_R], \tag{4}
\]

with \( g(\mathbf{x}, \zeta, t, \tau) = (2\pi \sigma^2)^{-3/2} \text{exp} (-|\mathbf{x} - \zeta|^2/2\sigma^2) \) is the fundamental solution of the heat equation with time dependent variance \( \sigma(t-\tau) = \sqrt{2\nu(t-\tau)} \).

The singular part of the vorticity field is not neglected but is accounted for at later times when the singular field had enough time to diffuse and reach length-scales comparable with the grid size. Given its smoothness properties the field \( \zeta_R(\mathbf{x}, t) \) can be represented on a discrete grid, provided the grid size \( \Delta \) is comparable with the smallest scale of the field \( \sigma_R(\epsilon_R) \) thus achieving the coupling with the carrier phase. In fact, the vorticity field given by
eq. (4) provides the regularized disturbance produced by a small spherical particle experiencing the drag force $D(t)$.

In the left panel of figure (2) we exploit the potential of the ERPP in dealing with actual turbulent flows. Here we present the data of an homogeneous shear flow at a Taylor Reynolds number of $Re_\lambda = 60$. The carrier phase is resolved by using $N_x \times N_y \times N_z = 256 \times 256 \times 128$ Fourier modes in a $4\pi \times 2\pi \times 2\pi$ periodic box. The flow is laden with $N_p = 2.200.000$ inertial particles with diameter $d_p = 0.1\eta$. The particle to fluid density ratio is $\rho_p/\rho_f = 1800$ corresponding to a particle Stokes time $\tau_p = (\rho_p/\rho_f) d_p^2/18\nu$ equal to the Kolmogorov time scale $\tau_\eta$, i.e. $St_\eta = \tau_p/\tau_\eta = 1$. The mass load of the disperse phase is $\Phi = 0.4$ where $\Phi$ is the ratio between the mass of the disperse phase and the carrier fluid. In the right panel of figure (2) we present a snapshot of the particle position in a $xy$ plane containing the mean flow. As expected particles with $St_\eta = 1$ are characterized by small scale clusters. Note also the preferential alignment of the aggregates according to the principal strain direction of the mean flow which is the signature of the small scale anisotropy of the clusters. In the context of the ERPP methodology we are able to compute in a closed analytical form the forcing operated by the particles on the fluid which is reported as a contour plot in the figure.

In the right panel of (2) we present an snapshot of the particle configuration in a turbulent round jet operated at a Reynolds number of 1500. The carrier flow is resolved in a cylindrical domain $2\pi \times 17R \times 30R$ in the azimuthal, radial and axial direction respectively by means of a standard staggered finite difference scheme as appropriate for incompressible flows. The jet inlet is provided by a companion simulation of a turbulent pipe flow which allows for realistic inflow conditions. The particles are injected at the inlet with a velocity matching the local fluid velocity. The mass loading, now defined as the ratio of particle-to-fluid mass throughput, is 0.4.

In the present contribution we will provide a detailed analysis of the turbulence modulation in the limit of $d_p/\eta \to 0$ by comparing the results obtained with the ERPP against the particle-in-cell approach [3, 5].

References


Figure 2: Left: Snapshot of the instantaneous particles position and corresponding intensity of the forcing on the fluid (contour plot) in a thin slice along the \(xy\) plane. The mean flow \(Sy\) is in the \(x\) direction from left to right. Right, snapshot of the particle configuration and instantaneous intensity of the fluid axial velocity (contour plot).
Particle statistics in turbulent channel flows with wall-roughness.

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Particle dynamics results in turbulent channel flows characterized by flat and rough walls will be shown in our talk. The two different flat and rough channel configurations laden with particles have been analyzed by means of Direct Numerical Simulation (DNS) to fully resolve the complex and multi-scale three-dimensional turbulent flow. Particle deposition and resuspension mechanisms at the wall turbulent flows are dominated by the coherent vortical structures arising in the inner region. These turbulent structures, which control the turbulent regeneration cycles, are strongly affected by the roughness of the wall. Particle dynamics in flat channels is characterized by a classical phenomenology named turbophoresis consisting in the preferential particle accumulation at the wall. Turbophoresis is investigated in a quantitative way as a function of the particle inertia. We show that wall roughness inhibits particle turbophoresis at the wall resulting in an increase of the particle mass flux through the channel section with respect to the flat configuration. Particle statistics, in term of mean particle concentration and probability density function of wall-normal particle velocity, show that the roughness produces a completely different scenario compared to the classical smooth wall, see [1] for a more detailed description.
High-performance computing for Volcanic ash plumes: turbulence, heat transfer and particle dynamics.

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We have developed a compressible multiphase flow model to simulate the three-dimensional dynamics of turbulent volcanic ash plumes. The model describes the eruptive mixture as a polydisperse fluid, composed of different types of gases and particles, treated as interpenetrating Eulerian phases. Solid phases represent the discrete ash classes into which the total granulometric spectrum is discretized, and can differ by size and density. The model is designed to quickly and accurately resolve important physical phenomena in the dynamics of volcanic ash plumes. In particular, it can simulate turbulent mixing (driving atmospheric entrainment and controlling the heat transfer), thermal expansion (controlling the plume buoyancy), the interaction between solid particles and volcanic gas (including kinetic non-equilibrium effects) and the effects of compressibility (over-pressured eruptions and infrasonic measurements). The model is based on the turbulent dispersed multiphase flow theory for dilute flows (volume concentration $\leq 0.001$, implying that averaged inter-particle distance is larger than 10 diameters) where particle collisions are neglected. Moreover, in order to speed up the code without losing accuracy, we make the hypothesis of fine particles (Stokes number $\leq 0.2$, i.e., volcanic ash particles finer than a millimeter), so that we are able to consider non-equilibrium effects only at the first order. We adopt LES formalism (which is preferable in transient regimes) for compressible
flows to model the non-linear coupling between turbulent scales and the effect of sub-grid turbulence on the large-scale dynamics. A three-dimensional numerical code has been developed basing on the OpenFOAM computational framework, a CFD open source parallel software package. The code has been tested on a variety of different numerical benchmarks, stressing all the physical aspects we want to resolve. Benchmarks demonstrate that the model is able to capture important non-equilibrium phenomena in gas-particle mixtures, such as particle clustering and ejection from large-eddy turbulent structures, as well as compressibility and thermal effects. A quantitative assessment of the reliability of Direct Numerical Simulation (DNS) and LES results with respect to modeling approximations and numerical errors has been carried out by comparing numerical results to experimental and computational studies of homogeneous, isotropic turbulence. In such a simplified geometry, the numerical solver is able to accurately reproduce the turbulent spectrum and the so-called energy cascade. The parallel efficiency on high-performance computing platforms exceeds 80% of numerical simulations. Other numerical benchmarks have been performed, such as the 2D lid-driven cavity, the natural convection in a square enclosure, the stratified mixing for a dam-break problem and the forced plume in an experimental setting. All these tests have given excellent results, in agreement with the data commonly found in the literature. Finally, the model is applied to simulate the three-dimensional dynamics of volcanic plume dynamics and demonstrate that gas-particle non-equilibrium phenomena have a significant impact on turbulent structures and can affect the entrainment rate and the subsequent atmospheric dispersal of volcanic ash.
Bubble dynamics and related acoustics

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The motion of a bubble of gas and vapour in an isochoric, inviscid liquid is numerically investigated in free space or in presence of a free surface and a gravitational force. The corresponding acoustic emission is evaluated. The liquid is at rest at the initial time, so that the subsequent flow is irrotational. The bubble motion is described in terms of the velocity potential, which is evaluated by means of an integral representation and the solution of an integral equation on the bubble boundary and the free surface. The pressure inside the bubble is assumed uniform and its value at time \( t \) is related to the bubble volume \( \mathcal{V} \) by the state equation

\[
p_B(t) = p_V + p_{G0} \mathcal{V}(0)/\mathcal{V}(t),
\]

\( p_V \) and \( p_{G0} \) being the vapour and gas pressure at \( t = 0 \), respectively. The corresponding pressure on the liquid face of the bubble boundary \( \mathcal{B} \) follows as

\[
p(z; t) = p_B(t) - 2S/R_m(z; t),
\]

\( S \) being the surface tension and \( R_m \) the mean curvature radius at the point \( z \in \mathcal{B} \). Once the pressure on the bubble boundary is known, the Bernoulli law is used to integrate the boundary values of the potential.
Discrete and continuous models for pedestrian movements

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This talk concerns the macroscopic model introduced by Andreianov, Donadello and Rosini for pedestrian evacuating a narrow corridor through a single exit. Starting from the classical scalar LWR model, we reproduce the gradual fall in the efficiency of the exit due to congestion by imposing that the flux at the exit satisfies a non–local constraint which depends on the density of pedestrians on a left neighbourhood of the door. The constraint function is exogenous and has to be determined together with the fundamental diagram from empirical data.

In [1] we prove the well–posedness of the Cauchy problem with Lipschitz non–local constraint by a procedure that combines the wave–front tracking algorithm with the operator splitting method. In [2], also in collaboration with Razafison, we study the Riemann problem in the case when the constraint function is merely piecewise constant. In the recent work, [3], we adapt to our framework the finite volumes scheme in [4] and [5], we validate it against explicit solutions, then we show that our model can reproduce phenomena as Faster is Slower and Braess’ paradox.

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1. Andreianov B., Donadello C. and Rosini M. D., 2013, *Crowd dynamics and conservation laws with non–local constraints and capacity drop*, accepted for publication in MMMAS.


Macroscopic modelling and simulations of crowd dynamics

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We consider two macroscopic models of crowd dynamics describing the evolution of the density of pedestrians in two space dimensions. The first one, introduced by Hughes [1], consists of a scalar conservation law closed with a speed-density relation. The second, proposed by Jiang et.al. [2], is a higher-order model given by the Euler equations for isentropic gas dynamics with relaxation source term and closed with a phenomenological law for the acceleration of pedestrians. Both systems take into account that pedestrians seek to minimize the path length towards their destination but temper their estimated travel time by avoiding high densities. This is obtained by coupling the above equations with the eikonal equation with a density dependent running cost function. The gradient of its solutions indicates the desired direction of motion of pedestrians.

We first provide a comparison between the two models regarding their ability of reproducing complex dynamics of crowd motion such as formation of stop-and-go waves and clogging at bottlenecks. Then we consider only the second order model and analyze the dependence of the behaviour of its solutions on some of the parameters of the system. In particular, we focus on the effect of the strength of the internal repealing forces. Finally, we study the optimization of the evacuation from a room through a narrow exit. Adapting the hypothesis of the inverse Braess paradox [3], we present some cases in which placing obstacles in front of the door prevents from blocking and decreases the evacuation time.


On the Hughes model for pedestrian flows: including local effects

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The Hughes model for pedestrian flow is based on the assumption that people want to minimize their travel time but try to avoid regions of high density. Local effects such as limited vision are not included in the model; the overall density of the crowd is known to every agent. We present a modification of the Hughes model to include local effects. We discuss modeling aspects on the micro- and macroscopic level as well as the efficient numerical simulation of the proposed models. Finally we illustrate the behavior of the modified model with various numerical experiments.
On the CR model and its applications at the bottlenecks

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The CR macroscopic model was introduced in [2] and its assumptions were later qualitatively validated in [4]. We start from the basic assumptions for its construction and show that Laxian shocks can not describe the raise of panic among pedestrians.

We show then how to apply the model to reproduce phenomena typical in crowd dynamics, namely the capacity drop at the bottlenecks [1], the faster is slower effect [3] and the Braess paradox [5].
Bibliography


Mean field games with nonlinear mobilities in pedestrian dynamics

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

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This communication refers to the modeling of crowd dynamics presented in [3]. The model consists in a scalar conservation law coupled with an eikonal equation, meant to describe the motion of pedestrians in a densely crowded region. We consider this model on a bounded one-dimensional domain, with zero-density boundary conditions. Therefore, the ending points represent the exits of the domain. The discontinuity locus of the gradient of the solution to the eikonal equation depends nonlocally on the solution to the conservation law, leading to an interesting mathematical problem. We show how to deal successfully with this situation under suitable assumptions on the initial data, leading to an existence result of discontinuous solutions for the model above.


Modeling Crowd Dynamics within the Framework of FPT7 Projects

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This communication refers to the modeling of crowd dynamics by kinetic theory methods where interactions are modeled by theoretical tools of stochastic games. The theoretical approach and some applications [1],[2],[3] are referred to specific requirements of projects of the European Union, where the main one consists in developing approaches suitable to capture the complexity features, including social behaviors, of the crowd viewed as a living system.

International Projects: EVAQUATE Dynamics of crowds in panic conditions, Started April 2013. SAFECITI Simulation Platform for the Analysis of Crowds Behaviour in Urban Environments with Training and Predictive Capabilities, (Started March 1, 2014)


Modeling rationality to control self-organization of crowds

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In this talk we present some mathematical models for pedestrian crowds, in which different degrees of rationality can be used by individuals when planning their path [2].

From the mathematical point of view, the pedestrian flow is described by a 2D continuity equation with nonlocal flux, in the spirit of multiscale model approach presented in [1]. On the other hand, rationality is included into the model by means of a suitable control problem that each walker has to solve to decide how to move. In particular, when each individual is capable to forecast the long term effects of their choices (highly rational behavior), the two problems are fully coupled and we end up with a first order mean field game [3].

Theoretical and numerical results will be presented to highlight the different behaviors of pedestrians, depending on the amount of information they can use, and to suggest that environment design could be exploited to get a “good” behavior even in the case of incomplete information and limited predictive capabilities.


Models and applications of conservation laws
Initial-boundary value problems for transport equations with rough coefficients

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I will be concerned with existence and uniqueness results for transport equations with weakly differentiable coefficients. The fundamental papers by Di Perna and Lions [4] and by Ambrosio [1] establish well-posedness of the Cauchy problem for transport equations with Sobolev and BV (bounded total variation) coefficients, respectively. This analysis has relevant applications to the study of several nonlinear partial differential equations, like for instance hyperbolic systems of conservation laws in several space dimensions [2].

My talk will aim at discussing existence and uniqueness results concerning solutions of initial-boundary value problems for transport equations with BV (bounded total variation) coefficients. I will also exhibit counter-examples showing that, as soon as the BV regularity deteriorates at the domain boundary, uniqueness is in general violated.


Rigorous derivation of the
Lighthill-Whitham-Richards model from the
follow-the-leader model as many particle limit

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We prove that the unique entropy solution to the macroscopic Lighthill-Whitham-Richards model for traffic flow can be rigorously obtained as the large particle limit of the microscopic follow-the-leader model, which is interpreted as the discrete Lagrangian approximation of the former. More precisely, we prove that the empirical measure (respectively the discretised density) obtained from the follow-the-leader system converges in the 1-Wasserstein topology (respectively in $L^1_{loc}$) to the unique entropy solution of the Lighthill-Whitham-Richards equation in the Kruzkov sense. The initial data are taken in $L^\infty$ with compact support, hence we are able to handle densities with vacuum. Our result holds for a reasonably general class of velocity maps (including all the relevant examples in the applications) with possible degenerate slope near the vacuum state. The proof of the result is based on discrete BV estimates and on a discrete version of the one-sided Oleinik-type condition. In particular, we prove that the regularizing effect “$L^\infty$ to BV” is intrinsic of the discrete model.
In this talk we shall consider an incompressible flow interacting with a boundary without assuming that the initial datum satisfies the no-slip condition at the boundary. A typical case when this situation occurs is the impulsively started disk. Other instances widely studied in the literature are when a vortical configuration, which is a steady solution of the Euler equations (like the thick core vortex or the vortex array), is assumed to interact instantaneously with a solid boundary.

Focusing our analysis on the Navier-Stokes equations on a half-space, we shall construct the initial-boundary layer corrector in the form of a Prandtl solution with incompatible data. This corrector is the first term of an asymptotic series that we shall prove to approximate, in the zero viscosity limit and for a short time, the Navier-Stokes solutions. Assuming analytic regularity in the tangential direction, we shall prove that this time does not depend on the viscosity.
From computer aided geometric design to industrial CAD modeling and simulations
Compatible discretizations based on hierarchical splines

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Isogeometric analysis is an emerging technology that intends to advance towards the integration of CAD and CAE technologies. The idea is, invoking the isoparametric concept, to use the same kind of basis functions for the geometry description given by CAD and the test and trial spaces in the discrete problem to be solved by CAE. The functions most commonly used up to now are (rational) B-splines and their non-tensor-product generalizations, such as T-splines and hierarchical splines.

By abandoning the isoparametric concept, it is possible to extend isogeometric analysis to the definition of discrete differential forms based on spline spaces. This kind of discrete spaces are useful for compatible discretization in computational electromagnetics and fluid mechanics, for instance, and they can be seen as a generalization of edge and face elements. In this talk I will present the definition of differential forms based on hierarchical splines, extending the result of previous papers to the non-tensor-product setting.
We propose a new sketch-based modeling paradigm where the creation of 3D models is automatically inferred from a 3D irregular curve network directly drawn by the user into a virtual 3D space. The user traces the 3D curve network using a natural user interface that mimics the free-hands drawing, which most users are familiar with. At this aim, we introduce a low cost, low power, wireless pen-like device, the SmartPen. The SmartPen is used to draw the style lines of the object to be modeled in the virtual space. Starting from the traced 3D curves, the system automatically reconstructs the sketched surface through an interactive optimization approach, finding the smooth subdivision surface which best fits the traced 3D curve network. The SmartPen also provides interactive capabilities to support the modeling process, introducing facilities for navigation and editing of the virtual scene. Moreover, real-time visual feedback is provided to the user to ease the overall experience. Various case tests are presented to demonstrate the effectiveness of the system in enabling the concurrent acquisition of the 3D curve network and the modeling of the underlying surface.
A spatial rigid body motion can be described in terms of the trajectory of a distinguished point of the body and the variation of an orthonormal frame, specifying the orientation of the body along this trajectory. Such a description essentially decomposes the spatial motion into translational and orientational components. Typically, the first component is straightforward, while the second one can pose difficulty. It is then important to be able to accurately associate a suitable frame to each point of the curved trajectory. Typical operations in this context may involve curvilinear abscissa identification, offsets computation, and also moving frame construction. Using classical polynomial/rational representations, these quantities can be non-rational and, consequently in commercial design applications they are usually approximated. In order to facilitate the construction of (constrained) interpolation/application algorithms, certain classes of polynomial/rational curves with a specific algebraic-geometric structure have been widely investigated. By focusing on the description of a camera moving along a spatial path while imaging a stationary object, a special family of frames (called directed) have been recently introduced. In particular, the rotation-minimizing property has been investigated.

In this talk, interpolation methods for constructing rational curves with rational directed rotation-minimizing frames are discussed.
Geometric Modeling for Turbine Engine Design

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The overall design of modern turbine engines is one of the most challenging tasks in today's engineering world comprising newest technologies in engineering design and simulation, material science and complex manufacturing processes. Within the design process, the capability of fast and robust geometric algorithms for an automatic 3D shape optimization of turbine and compressor blades is a key technology for creating highly efficient engines minimizing flow losses.

The mini-symposium talk will introduce MTUs geometric modeling and processing software COBRA and the Marie Curie research project EXAMPLE, both focusing on bridging the gap between advanced techniques in computer aided geometric design and innovative industrial applications. COBRA combines geometric algorithms with a modern software architecture providing visualization, data management and user interfaces for a real industrial software. Currently, it is deployed for the aerodynamic shape design of engines like the PW1100G for the Airbus A320neo. EXAMPLE focuses on the scientific field of geometric techniques, especially on developing hierarchical spline spaces, and their application within the industrial environment at MTU. Therefore, we will present first results for the adaptive CAD model (re-)construction with the so-called truncated hierarchical splines and the integration of the adaptive modeling tool into CAD systems that comply with the current NURBS standard.