C U R S O S E C O N G R E S O S

19th European Conference on Mathematics for Industry

Santiago de Compostela (Spain)
June, 13-17, 2016

ECMI 2016
Book of Abstracts

Edited by
Peregrina Quintela
Patricia Barral
Dolores Gómez
Francisco-José Pena
Jerónimo Rodríguez
Pilar Salgado
Miguel E. Vázquez-Méndez

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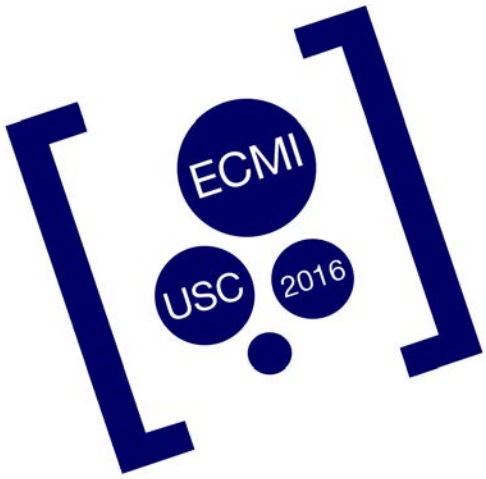

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Preface

This volume contains the abstracts of the lectures given at the 19th European Conference on Mathematics for Industry (ECMI 2016), held in Santiago de Compostela on 13-17th June 2016.

The conference is organized every two years with the aim to reinforce the interaction between academy and industry, leading to innovation in both fields. ECMI conferences also encourage industrial sectors to propose challenging problems where mathematicians can provide insight and new ideas. These conferences are one of the main forums where significant advances in industrial mathematics are presented, bringing together prominent figures from business, science and academia to promote the use of innovative mathematics to industry.

ECMI 2016 is jointly organized by the Department of Applied Mathematics at the Universidade de Santiago de Compostela (USC) and the Spanish Network for Mathematics & Industry (math-in). In this 19th edition a wide variety of applications will be presented ranging from problems in Electronics (15%), Energy and Environment (14%), Mechanics and Mechatronics (12%), among industrial sectors with the highest number of talks.

When classifying the talks according to the societal challenges of the EU Framework Program for Research and Innovation H2020 is observed, 14% of them fall into the challenge Climate action, environment, resource efficiency and raw materials; 13% to the Health, demographic change and wellbeing; while a 12% belong to the Europe in a changing world - inclusive, innovative and reflective societies.

The ECMI 2016 scientific program consists of 10 plenary talks by some of the leading researchers in industrial mathematics, 40 mini symposia in specific areas covering a wide variety of recent developments, and 19 sessions of contributed talks. In short, we will have a total of 306 presentations distributed along 5 days with 8 parallel sessions per day. In these presentations there are, directly or indirectly, involved about 50 companies that, in one way or another, have funded the research presented to meet their specific demands. Also many cases success stories from established collaborations with industry will be presented. Special mention must be made to the dissemination event “The mathematical way to the Oscars” to be held in the Auditorium of Abanca (Pazo de Ramiráns), which will feature the participation of an invited speaker from academia and two representatives from companies familiar with the use of mathematical technology in movie production. The conference program also pays special attention to establishing discussion forums in various fields, such as mathematics in the H2020 programme, Master’s programmes related with Industrial Mathematics, or Study Groups as a tool for dissemination and promotion of mathematical technology.

The abstracts are classified into four sections: Plenary lectures, ECMI awards and special lectures, minisymposia and contributed talks.

This edition will count with 350 participants from 40 countries, involving the five continents. The majority of the attendees come from 26 European Countries but there are also representatives from Australia, America (Canada, Mexico and USA), Africa (Nigeria, Sudan, Tanzania and Uganda) and Asia (China, India, Israel, Philippines and Japan). The Spanish participation is the largest representing 25% of the total, closely followed by Germany with 20%.

ECMI 2016 received generous support from the ECMI, the Universidade de Santiago de Compostela, the Spanish Network for Mathematics & Industry , the Spanish Ministry of Economy and competitiveness, the Naval Research Office of United States of America, the Thematic Network of Mathematics & Industry, the Technological Institute of Industrial Mathematics, and the Galician Network of Industrial Mathematics. We also have had the collaboration of several institutions or companies like GDI, Iberia, Renfe, Springer, Xacobeo Galicia, and Santiago Turismo. We would like to thank all of them; their support has contributed to the successful of this event and was crucial allowing many young researchers to participate in ECMI 2016.

The Organizing Committee wish to thank all participants for their contributions and attendance, without whom there would have been no conference. Special thanks to the Scientific Committee, the invited speakers, the organizers of special sessions and the chairs and assistants of the different sessions.

Finally, we would like to express our gratitude to Elisa Eiroa, manager of the research group in Mathematical Engineering (mat+i), Fe Sampayo, technology translator in math-in, Manuel Porto, secretary of the Department of Applied Mathematics, and Carlos Grela, technical assistant of the mat+i group, for their help organizing this event. Furthermore we would like to thank the Faculty of Biology and the Faculty of Mathematics, which provided us with spaces for this conference.

We hope that you will find the 19th edition of ECMI interesting, stimulating and a great experience altogether. Santiago de Compostela, June 2016

Peregrina Quintela,

ECMI 2016 Organizing Committee Chair
On behalf of the ECMI 2016 Organizing Committee

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Boundary element method for electromagnetic compatibility problems

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Electromagnetic immunity problems represent a major issue in aeronautic industry and concern a wide variety of phenomena and threats: Lightning Indirect Effects (LIE), High-Intensity Radiated Fields (HIRF), antenna coupling, wireless networks... The design of electromagnetic protection is a difficult task with multiple constraints: weight, cost, delays, life-cycle management... The extensive use of light-weight composite and smart materials, the increasing complexity of onboard systems, the uncertainties (related to material properties, manufacturing, ageing...) make the problem very complex. It is essential to boost simulation capabilities in order to safely introduce innovations in the aircraft design and move to robust design and margin management.

These industrial needs pose significant challenges for numerical modelling:

- deal with a very large frequency band, starting from DC up to several Gigahertz. For time domain solvers, that represents a huge number of time steps, dispersion and late time instability issues, while frequency domain solvers may be subject to instability in the low frequency regime. Loop-tree decomposition can be used for this issue but it is notoriously difficult to apply for multi-domain problems;
- estimate and implement reduced models (wires, slots, equipments, generators...) in 3D solvers;
- handle multi-partner collaborative simulation and design optimisation: domain decomposition techniques and ability to couple 3D-models with complex nonlinear circuit models of equipments...
- efficiently handle transmission conditions (including skin effect) and evaluate low levels of currents and fields inside closed cavities;
- take into account geometric and data singularities. A combination of *a priori* and adaptive meshing procedures based on *a posteriori* error estimates is required for robust (engineer-independent) simulations;
- reliable and efficient model reduction for parametric studies and uncertainty management;
- model size (number of degrees of freedom) requires efficient fast and parallel solvers.

We show how these issues can be addressed by a frequency domain integral equation method. In particular, we show how a multi-trace BEM formulation can solve both the low level in cavities and the low frequency instability issues. We present some industrial numerical examples.

Keywords: Integral equation, BEM, multi-trace formulation, a posteriori estimates, adaptive mesh refinement, EMC, LIE, HIRF.
Acknowledgments. This work is supported by Airbus Group, the French National Research Agency (ANR) and the French Procurement Agency (DGA).

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Mathematical modelling of lithium ion batteries

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A framework is presented for modelling the physical and chemical dynamics of a lithium-ion battery using the method of multiple scales to derive a macroscopic model from a detailed electrode microstructure [2, 3]. The result is a porous electrode model similar in flavour to the standard model of Newman [1], but in which the macroscopic parameters such as permeability are directly related to the microscopic electrode structure.

The model includes both electrokinetic transport phenomena and mechanical deformation due to electrode swelling, and is thus able to predict local mechanical stresses. These in turn may lead to cracking with a resulting degradation of battery performance.

Keywords: Homogenisation, electrochemistry, porous media, growth, mechanics.
Acknowledgments. Supported by EPSRC research project EP/I017070/1.

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Mathematical modeling of membrane filtration

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Membrane filters – essentially, thin sheets of porous medium which act to remove certain particles suspended in a fluid that passes through the medium – are in widespread industrial use, and represent a multi-billion dollar industry in the US alone. Major multinational companies such as W.L. Gore & Associates, and Pall Corporation, manufacture a huge range of membrane-based filtration products, and maintain a keen interest in improving and optimizing their filters. Membrane filtration is used in applications as diverse as water purification; treatment of radioactive sludge; various purification processes in the biotech industry; the cleaning of air or other gases; and beer clarification. While the underlying applications and the details of the filtration may vary dramatically (gas vs liquid filtration; small vs large particle removal; slow vs fast throughput; rigid vs deformable particles), the broad engineering challenge of efficient filtration is the same: to achieve finely-controlled separation at low power consumption.

The desired separation control is to remove only those particles in a certain size range from the input flow (often referred to as "feed"); and the obvious resolution to the engineering challenge would appear to be: use the largest pore size and void fraction consistent with the separation requirement. However, these membrane characteristics (and hence the filter's behavior and performance) are far from constant over its lifetime: the particles removed from the feed are deposited within and on the membrane filter, fouling it and degrading the performance over time. The processes by which this fouling occurs are complex, and depend strongly on several factors, including: the internal structure of the membrane; the flow dynamics of the feed solution; and the type of particles in the feed (the shape, size, and chemistry affects how they are removed by the membrane).

Though the fouling literature is extensive, a complete and coherent predictive framework that can realistically describe all fouling modes of a membrane filter is still lacking. A recent review by Iritani [1] concludes by noting that "... further development of simple yet effective mathematical models for elucidating the complicated pore-blocking phenomena in membrane filtration would be highly desirable for guiding decisions on the optimal choice of the membrane and membrane-cleaning strategy in industrial use."

In this talk we will describe some of our recent and ongoing work on first-principles modeling of membrane filtration and fouling [2, 3]. Particular emphasis is paid to how membrane filter design (*e.g.* permeability gradients across the membrane) can significantly affect filtration efficiency, as measured by (i) total throughput over a filter lifetime, and (ii) proportion of particles removed from the feed.

Keywords: Membrane filter, porous medium, fouling, permeability.
Acknowledgments. Partially supported by the National Science Foundation under grants DMS-1261596 and DMS-1153954, and by Pall Corporation. Stimulating discussions with Ian Griffiths (University of Oxford), Anil Kumar (Pall Corporation), Giles Richardson (University of Southampton) and Tom Witelski (Duke University) are gratefully acknowledged.

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Geometrical multi-scale modeling of liquid packaging system: an example of scientific cross-fertilization

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Geometrical multi-scale modeling that comprises the coupling of differential models operating at different spatial dimensions (3D, 1D, 0D, for instance) have proved very successful in the simulation of the human cardiovascular system [1, 2].

The long-lasting experience in such type of modeling is here exploited in a very different context, that is the numerical modeling of packaging systems for liquid food products. Indeed, this application shares many common features with the flow in the cardiovascular system, in particular strongly coupled fluid-structure interactions (FSI), the presence of flow in pipes coupled with both complex three-dimensional geometries and lumped (zero-dimensional) models. The final objective of this numerical investigation is the development of an efficient tool for the simulation of the pressure wave propagation through the different components of the packaging system.

In this talk, we will present a family of models that can be applied to this type of problems, their numerical implementation and numerical results that show the effectiveness of the procedure adopted for the solution of a real industrial application.

The work is an example of contamination of ideas between different applications and is the result of a fruitful collaboration among academic and industrial researchers.

Keywords: Fluid-structure interaction, geometrical multi-scale.
Acknowledgments. This research project was supported by Tetra Pak Packaging Solutions S.p.A.

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Semiparametric prediction models for variables related with energy production

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The "Semiparametric Statistical Inference" was object of study in last decades with new methodological advances and nice applications.

In this talk, we will present different semiparametric dynamic regression models designed for the prediction of variables related with energy production. Mainly, with variables associated with the effects of the pollution and the demand of energy.

In the first part of the talk, we will review different models developed throughout the years thanks one extensive collaboration between the Department of Statistics and Operation Research of the University of Santiago de Compostela and Endesa Generation, S.A., in Spain. Starting with one first study (García-Jurado et al (1995)), several predictive methods were considered for the forecasting of future values of SO_2 and NO_x. Neural Networks and models with functional predictors are examples of the different developed statistical tools, which were included in one "Supplementary Control System of Air Quality" for one power station in the northwest of Spain.

In the second part of the talk the revision is related with models for variables associated to the electricity consumption. A new step-wise method using one combination of the modern "distance correlation" (Szekely et al. (2007)) with selection criteria of general functional covariates to be used in generalized additive models (Febrero-Bande and González-Manteiga (2013)) is given.

Keywords: Semiparametric prediction models, Environmental Sciences, Energy.
Acknowledgments. Partially supported by Project MTM2013-41383P from the Spanish Ministry of Economy and Competitiveness.

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Emergent behaviour in T-cell immune response

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Humans are able to implement efficient immune responses to address pathogenic challenges. It is truly remarkable that such actions arise out of individual decisions made by each single cell according to information provided by her immediate neighbourhood as interpreted through her membrane receptors only. In particular, no central coordination organ supervises the resulting population behaviour. Moreover, the number of individual choices for the involved cells is rather limited, and usually reduces to deciding between cell division, cell death by apoptosis and differentiation into a new type of cell. In spite of the local nature of any such decision, a coordinated response is observed at the population level, which can be seen as an emergent property of the underlying dynamics.

In this lecture a particular example of such emergent behaviour, namely T-cell mediated immune response to acute infection, will be discussed. More precisely, a minimal model will be presented to explain an intriguing feature of such response, namely the onset of a delayed clonal contraction. This term refers to the fact that a) effector T-cells continue to be produced in high numbers well after the pathogen numbers have become negligible, and b) later on, most of the large T-cell population thus generated is eliminated by apoptosis, except for a small percentage of already trained individuals that are preserved as memory cells. These will thus be in place to mount a response, should a similar pathogenic invasion takes place in a near future. Interestingly, a similar approach allows to discuss possible mechanisms for T-cells to tell friend from foe when facing antigenic stimuli, be it produced by their own body or having an external origin instead. To conclude, a number of generalizations and future research directions will be discussed.

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Mathematics of nonlinear acoustics: modeling, numerics, optimization

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High intensity ultrasound is used in numerous medical and industrial applications ranging from litotripsy and thermotherapy via ultrasound cleaning and welding to sonochemistry. We will highlight several mathematical and computational aspects related to the relevant nonlinear acoustic phenomena.

Physical and mathematical modeling of high intensity ultrasound and generally of nonlinear acoustics is still an ongoing process and a field of active research. The classical models of in this context are nonlinear wave equations exhibiting potential degeneracy as well as strong damping. Taking into account higher order effects leads to third or fourth order PDEs. An additional important issue is the coupling of acoustics to other physical fields, e.g., when focusing by a linearly elastic silicone lens immersed in the nonlinearly acoustic fluids, as typical for a widely used class of lithotripsy devices.
This is joint work with Irena Lasiecka (University of Memphis), Rainer Brunnhuber (Alpen-Adria-Universität Klagenfurt), Vanja Nikolić (TU München) as well as Petronela Radu (University of Nebraska at Lincoln)

In the simulation of high intensity ultrasound, a particular challenge due to nonlinearity and the presence of different wave lengths is efficient and robust time integration. For this purpose, a promising approach are operator splitting techniques exploiting the intrinsic structure of the equations. The original second or third order in time evolution equations are split into simple subproblems that can be solved by standard methods or even explicitely. Combination of such appropriately weighted subproblems by exponential operator splitting schemes leads to highly efficient time integration methods.
This is joint work with Vanja Nikolić (TU München) and Mechthild Thalhammer (University of Innsbruck)

Strictly speaking, acoustic sound propagation takes place in full space $\mathbb{R}^d$, or at least in a domain that is typically much larger than the region of interest Ω. To restrict attention to a bounded domain Ω, e.g, for computational purposes, artificial reflections on the boundary $\partial\Omega$ have to be avoided. This can be done by imposing so-called absorbing boundary conditions ABC that induce dissipation of outgoing waves. Here it will turn out to be crucial to take into account nonlinearity of the PDE also in these ABC.
This is joint wirk with Igor Shevchenko (Imperial College London).

Finally, we will discuss some practically relevant optimization problems in the context of nonlinear acoustics applications in lithotripsy. The optimal choice of ultrasound excitation via piezoelectric transducers leads to a boundary control problem; focusing high intensity ultrasound by a silicone lens requires shape optimization. For both problem classes, we will discuss the derivation of gradient information in order to formulate optimality conditions and drive numerical optimization methods.
This is joint work with Christian Clason (University of Duisburg-Essen), Vanja Nikolić (TU München), and Gunther Peichl (University of Graz)

References and discussion of some further aspects can be found in [1]

Keywords: nonlinear acoustics, splitting methods, absorbing boundary conditions, boundary control, shape optimization
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Optimization, modeling, and data sciences for energy systems

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For decades, power systems have been playing an important role in humanity. Industrialization has made energy consumption an inevitable part of daily life. Due to our dependence on fuel sources and our large demand for energy, power systems have become interdependent networks rather than remaining independent energy producers. This talk will focus on the problems arising in energy systems as well as recent advances in optimization, modeling, and data sciences techniques to address these problems. Among the topics to be discussed are emission constrained hydrothermal scheduling, electricity and gas networks expansion, as well as reliability analysis of power grid.

Keywords: optimization, modeling, power systems, smart grid, energy industry.
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The weighted least action principle: theory and applications

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The Optimal Transport problem, first formulated by Monge in 1781, has become a central theme in modern analysis [5]. It involves fascinating mathematics, poses great computational challenges, and has already met with many applications ranging from fluid mechanics [1], to economy and to medicine.

In my talk I shall review recent developments in this theory from an applied mathematician point of view. After introducing the key concepts, I shall discuss recent theoretical advances motivated by fundamental questions in wave propagation [2].

In particular I shall explain the connection between optimal transport and geometric optics for dispersive waves, and extensions of the classical optimal transport theory to dissipative systems and to singular solutions [4].

Finally, I shall review applications to practical problems in optics, including phase reconstruction and beam shaping [3].

Keywords: optimal transport; wave propagation; imaging optics; nonimaging optics.

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Snow business: scientific computing in the movies and the classroom

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New applications of scientific computing for solid and fluid mechanics problems include simulation of virtual materials for use in movie special effects and virtual surgery. Both disciplines demand physically realistic dynamics for materials like water, smoke, fire, and brittle and elastic objects. Separate new algorithms are required for each area. Teran will speak about the simulation techniques required in these fields and will share some recent results including: simulated surgical repair of biomechanical soft tissues; extreme deformation of elastic objects with contact; high resolution incompressible flow; and clothing and hair dynamics. He will also discuss a new algorithm used for simulating the dynamics of snow in Disney's animated feature film, "Frozen".

Keywords: numerical PDEs, computational solids, computational fluids, Particle-In-Cell, Material Point Method, computer graphics.
Acknowledgments.: Work was partially supported by NSF CCF-1422795, ONR (N000141110719, N000141210834), Intel STC-Visual Computing Grant (20112360) as well as a gift from Disney Research.

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ECMI awards and special lectures

Alan Tayler Memorial Lecture

This lecture was set up by the ECMI Council to honour Alan Tayler who died on January 28th 1995. Alan was one of the founding members of ECMI and was the third President in 1989. The Alan Tayler Lecture has been a key feature of the biennial ECMI conferences since 1996. The 2016 Alan Tayler Memorial Lecture will be given by **S. Jon Chapman** and will be entitled

Mathematical modelling of lithium ion batteries.

Anile-ECMI Prize for Mathematics in Industry

The Anile-ECMI Prize for Mathematics in Industry was established honouring Professor Angelo Marcello Anile (1948-2007) of Catania, Italy, consists of a prize of 2500 Euros and an invitation to give a talk at the ECMI 2016 conference.

The prize is given to a young researcher for an excellent PhD thesis in industrial mathematics successfully submitted at a European university in 2014-2016. The 2016 Anile-ECMI Prize for Mathematics in Industry is awarded to **Francesc Font** from the University of Limerik. Francesc will present at ECMI 2016 a talk entitled

Influence of substrate melting on the laser-induced dewetting of nanothin films

which is scheduled in the minisymposium *MS03: Moving boundary problems in industrial applications*.

Hansjörg Wacker Memorial Prize

The Hansjörg Wacker Memorial Prize was established in memory of ECMI founding member Hansjörg Wacker (1939-1991), who was Professor of Numerical Mathematics at the Johannes Kepler University, Linz. The prize is jointly funded by ECMI and by a consortium of institutions from Linz which comprise the Industrial Mathematics Institute and the Institute of Computational Mathematics of Johannes Kepler University, and the Johann Radon Institute for Computational and Applied Mathematics of the Austrian Academy of Sciences. It consists of a prize of 1000 Euros and the invitation to attend the ECMI 2016 conference presenting his/her project as a contributed talk.

The prize is awarded for the best mathematical dissertation at the Masters level on an industrial project written by a student from an ECMI institution. The 2016 Hansjörg Wacker Memorial Prize is awarded **Elisa Riccietti** from the Università degli Studi Firenze. Elisa will present at ECMI 2016 a talk entitled

Numerical methods for optimization problems: an application to energetic districts

which is scheduled in the session of Contributed Talks *CT05: Optimization problems*.

Minisymposia

MS01: Spacetime models of gravity in space geolocation and acoustics

MS01: Spacetime models of gravity in apace geolocation and acoustics

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The geometrization of gravity has become one of the cornerstones of modern science having an impact on the industrial progress connected to many activities of daily life. In fact, in the last decades substantial research has been invested into post-Newtonian corrections for high-precision space geodesy and navigation [1, 2, 3, 4], as well as into the design of analogue models of gravity by making use of advanced optical and acoustic metamaterials (see e.g. [5, 6, 7]). Other present industrial procedures requiring very accurate timing show the need of innovative development of computationally efficient space-time models for use in space. In particular, these models become important in geolocation of passive radiotransmitters in space and to improve active space debris removal [8, 9, 10]. Moreover, acoustic metamaterials—artificially produced materials with exceptional properties not found in nature—provide the engineer with tools to fabricate acoustic devices with highly unusual features. However, the mathematical modelling of acoustic phenomena with curved background spacetimes not only poses challenges in engineering, but may also raise fundamental questions beyond their possible verification in the laboratory environment. This minisymposium is continuation of the ECMI 2014 Minisymposium "Spacetime Models of Gravity in Space Geolocation and Acoustics", so that it is dedicated to the last three topics just mentioned. The session starts with a contribution aimed to determine velocities and frequencies of emission of passive radiotransmitters in space by FDOA. The work is in line with previous works carried out at the University Carlos III of Madrid [11, 12, 13] with the collaboration of the Instituto de Matemática Multidisciplinar of the Universitat Politècnica de València. The speaker and title of the talk are

> Javier Clares. Universidad Carlos III de Madrid (Spain). *FDOA determination of velocities and emission frequencies of passive radiotransmitters in space.*

The following contributions form the last step in a series of recent works [14, 15]. This series is aimed to help increase the accuracy of the space based APT systems endowed with very narrow laser beams e.g. for active space debris removal. In particular, the second contribution shows the results of several experiments obtained by numerically solving the equations of the first contribution, and is the result of a cooperation between Gregorio Millan Institute from the University Carlos III of Madrid and the Institute for Analysis and Scientific Computing from Vienna University of Technology, and the third, between Gregorio Millan Institute and personnel of ALTEN. The speaker and title of the first talk are

> Jose M. Gambi. Universidad Carlos III de Madrid (Spain). *Non-linear post-Newtonian equations for the motion of designated targets with respect to space based APT laser systems.*

The speaker and title of the second talk are

> Maria L. García del Pino. Universidad Carlos III de Madrid (Spain). *Post-Newtonian corrections to the Newtonian predictions for the motion of designated targets with respect to space based APT laser systems.*

The final contribution is dedicated to the emerging field of transformation acoustic. Here, in particular the focus is on modelling acoustic wave propagation in 2D spaces of constant curvature with the help of a variational principle. The contribution on this topic is led by the Universitat Politècnica de València [16, 17, 18], and so far, one previous work includes the cooperation of members of the Institute for Analysis and Scientific Computing from Vienna University of Technology [19]. The speaker and title of the talk are

Michael M. Tung. Universitat Politècnica de València (Spain). *Acoustics in 2D spaces of constant curvature.*

Keywords: APT laser systems, Acoustic metamaterials, transformation acoustics, Geolocation, post-Newtonian relative orbital motions, NoSQL.

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FDOA determination of velocities and emission frequencies of passive radiotransmitters in space

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The two systems of Frequency Difference of Arrival (FDOA) equations here introduced are aimed to determine in real time the velocities of passive, i.e. non-cooperative, radiotransmitters at the emission instants, together with the frequencies of emission. The reference frame used is the Earth Centered Inertial (ECI) reference frame, and the equations correspond to the Newtonian and post-Newtonian approximations to the Schwarzschild field for the Earth surrounding space. The radiotransmitters may be placed on the Earth surface or in orbit about the Earth, and the computations can be carried on at the time the radiotransmitters are being located.

The equations are consistent with other equations in previous works, which are related, like this, to Geolocation. In fact, they have been derived by means of the same tools, which are the versions of Synge's world function most suitable to the scenarios considered on this occasion [1]-[6]. On the other hand, Synge's world function is used, because it has proved very efficient in many other scenarios, such as in Navigation (see e.g. [7]), and nowadays is considered as a universal tool (see e.g. [8]-[10]).

As a consequence we have that each system of FDOA equations may yield accurate solutions at the respective level of approximation, particularly if the locations have been determined by means of Time Difference of Arrival (TDOA) measurements. In fact, if these measurements are made by three GEO and two LEO satellites, and the arrival frequency measurements are made by the same LEO and two of the three GEO satellites, the post-Newtonian corrections to the Newtonian solutions due to the differences of the Earth tidal effects at the receivers and to the gravitational signals' time delays can be computed.

Keywords: Geolocation, FDOA, Earth post-Newtonian framework.

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Non-linear post-Newtonian equations for the motion of designated targets with respect to space based APT laser systems

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The increasing presence of middle size debris objects about the Earth represents a serious threat of collision with satellites on active duty. This scenario set us before the goal of ablating these objects by means of space-based Acquisition, Pointing and Tracking (APT) laser systems. This is a real challenge, since, according to the catalogue of the US Space Surveillance Network (SSN), the average size of these objects ranges between 1 cm to 10 cm [1]. Hence the main dynamical issue previous to the implementation of the pointing directions with very narrow laser beams from the Line-of-Sight (LOS) directions is to accurately predict the motion of these targets with respect to the systems. The equations of motion introduced in this paper are aimed to help increase this accuracy. They are derived under the assumption that the structure of the Earth surrounding space is post-Newtonian, keeping thus consistency with previous works in Space Geodesy, Positioning, Navigation and Geolocation (see e.g. [2]-[7]). The equations are derived from Synge's equations of geodesics in Fermi coordinates [8]; they are non-linear and are the last step ahead up to the date of a sequence of equations that generalize the familiar equations of the geodesic deviation for the weak approximation to the exterior Schwarzschild field (see e.g. [9]). Thus, unlike these equations, whose coefficients are the values of the tidal potential at the positions of the APT systems, the coefficients of the equations introduced here are integrals of this potential, and of its spatial derivatives, taken along the straight line segments that, while orbiting, join the systems and the targets, as in [8]. Hence they are not only valid for targets close to the systems, but also, like the Newtonian equations, for distant targets. The equations are formulated in local Cartesian coordinates; therefore, they are primarily adapted for use with inertial guided APT systems. The suitability of these equations is numerically analyzed by means of appropriated tests in the ECMI 2016 contribution "Post-Newtonian corrections to the Newtonian predictions for the motion of designated targets with respect to space based APT laser systems". In addition, one contribution that introduces a graphical user-friendly interface for the resolution of these equations is also presented in this Minisymposium.

Keywords: Post-Newtonian equations, relative orbital motions, APT laser systems.

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Post-Newtonian corrections to the Newtonian predictions for the motion of designated targets with respect to space based APT laser systems

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Numerical solutions of the Newtonian equations for the Earth Centered Inertial (ECI) relative motions of designated targets with respect to space based laser Acquisition, Pointing and Tracking (APT) systems are used to estimate the short/long term differences between the ranging predictions provided by these equations and those provided by three systems of post-Newtonian equations. The first system describes the relative motions by means of the differences between the post-Newtonian equations for the ECI orbital motions of the targets and the APT systems in the Earth Schwarzschild field, thus resembling the procedure followed to derive the Newtonian equations; the second, by means of the linear approximation to Synge's equations for the relative motion in Fermi coordinates derived by Gambi et al. for this field [1, 2], and the third, by means of the equations introduced in the contribution "Non-linear post-Newtonian equations for the motion of designated targets with respect to space based APT laser systems" presented in this ECMI 2016 Minisymposium. Accordingly, the estimations are made under the following assumptions: (i) the geometrical structures of space-time about the Earth are those of the Newtonian and post-Newtonian approximations to the exterior Schwarzschild field, and (ii) the APT systems are inertial guided. To resemble actual scenarios, the systems are assumed to be onboard GEO satellites, and on LEO satellites that are in equatorial circular orbits about the Earth. In turn, the targets are assumed to be initially at short, and successively increasing distances from the systems.

From the simulations carried out in this work, we may reasonably conclude that for realistic distances the third system of equations, i.e. the non-linear system introduced in this minisymposium, is the most appropriate to correct the solutions derived with the Newtonian model for the laser links at practically any instant, even within the early stages of the integrations. The reasons that lead us to this conclusion are: (i) unlike for the terms in the linear system, the corrections due to the non-linear terms make the size of the total post-Newtonian corrections to fit perfectly well with the size of the gravitational corrections considered in the post-Newtonian approximation to the Schwarzschild field; and (ii) the underlying curved structure of space-time corresponding to this approximation becomes apparent through this system, since, unlike for the Newtonian method, there are significative differences between the predictions derived with it and those derived by means of the first system of equations. On the other hand, the corrections predicted by the non-linear system amount to quantities that increase along with the distance from the APT systems to the targets, as the integration time increases. In fact, these quantities become measurable shortly after the initial integration instants. Hence they can be taken into consideration to increase the pointing accuracy of the APT systems, because the size of the corrections may become larger than the size of many potential targets in the scenarios considered.

Keywords: Numerical simulations, relative orbital motions, Earth post-Newtonian framework.

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Acoustics in 2D spaces of constant curvature

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Spaces of constant curvature are maximally symmetric spaces, and from this property derives its vital importance in physics and engineering applications, such as *e.g.* the description of uncharged, perfect relativistic fluids [1] and standard cosmological models [2]. Moreover, in the past years, quantum mechanical phenomena in spaces of constant curvature have attracted the focus of intense investigation [3], raising critical fundamental questions beyond their possible experimental verification. However, the simulation of acoustic phenomena [4] in such spaces has so far been vastly neglected.

Among the most significant spaces of constant curvature are the n-spheres embedded in $(n+1)$-dimensional Euclidean space, denoted by $\mathbb{S}^n(K)$, where $K > 0$ is the curvature. Then, the corresponding m-dimensional spacetime consists of the Lorentzian manifold $\mathbb{R} \times \mathbb{S}^{m-1}(K)$, which is conformally flat.

In this work, we will consider a locally homogeneous and isotropic (2+1)D spacetime of Robertson-Walker type and therefore with underlying de Sitter space $\mathbb{R} \times \mathbb{S}^2(K)$. Modelling acoustic wave propagation in this curved background space can be shown to result from a simple variational principle for the acoustic potential [5, 6, 7]. We demonstrate how this approach yields a partial differential equation for the potential, connected to a harmonic time dependence and to a Sturm-Liouville problem for the radial isotropic coordinates, which can be tackled analytically. The conclusion contains a brief discussion of the expected wave predictions and comments on the design and implementation of such spacetime with suitable acoustic metadevices.

Keywords: transformation acoustics, curved acoustic spaces, conformally flat Lorentzian manifolds, acoustic metamaterials.
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MS02: Applied mathematics in stent development

MS02: Applied mathematics in stent development

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Coronary artery disease is a global problem and devising effective treatments is the subject of intense research activity throughout the world. Over the past decade, stents have emerged as one of the most popular treatments. Acting as a supporting scaffold, these small mesh devices are now routinely inserted into arteries where the blood flow has become dangerously restricted. Stents have evolved from bare metal scaffolds to polymer coated drug-delivery vehicles and, more recently, sophisticated fully biodegradable drug delivery configurations. Despite these advances, significant opportunities to improve on arterial stent design remain. The relative success of coronary artery stenting has led to the emergence of stenting technology for the carotid, neural and peripheral vasculature. In addition, the adaptability of the stent concept has opened horizons beyond the vasculature, with stent technology now being developed for, amongst others, pulmonary, gastro-intestinal and structural heart applications.

This mini-symposium will cover the development of innovative models to help industry optimise and improve the stent design, to identify the key parameters governing the behaviour of the system, to simulate the flow of plasma around complex stent geometries, to identify the drug release mechanism, and to help decrease the number of experimental studies, thereby saving time and money. As well as providing a platform for contributed talks from members of the newly formed ECMI special interest group '*Advancing the design of medical stents*', this mini-symposium is open to researchers with expertise in continuum mechanics, physiological flow modelling, structural and soft tissue mechanics, numerical analysis, mathematical biology and multi-objective optimisation, to name but a few.

Speakers:

S. McGinty. University of Glasgow (Scotland). *The role of mathematics in stent development.*

Abdul I. Barakat. Ecole Polytechnique (France). *Optimizing the performance of drug-eluting stents: simulations and experiments.*

T. T. N. Vo. University of Limerick (Ireland). *Mathematical models of drug release from polymer-free drug-eluting stents.*

G. Pontrelli. IAC-CNR, Rome (Italy). *Variable porosity coatings as a means of controlling drug release from stents.*

J. Escuer. University of Zaragoza (Spain). *Numerical simulation of drug transport in arterial wall under healthy and atherosclerotic conditions.*

Keywords: mathematical modelling, numerical simulation, stent development, controlling drug release.

The role of mathematics in stent development

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Stents are tiny scaffolds which are used to widen arteries where the blood flow has become restricted. The most common use of stents is in treating coronary heart disease. These stents are now typically coated with a drug to reduce inflammation and are therefore called drug-eluting stents (DES). Over the past decade, various generations have emerged which include biodegradable polymer coated, polymer-free and bioresorbable stents. Whilst current DES generally perform well, researchers across academia and industry are engaged in trying to design better stents which can address important concerns such as delayed healing and can be used in patients with more complicated disease.

Traditionally, a purely empirical approach has been adopted by manufacturers in designing new stents. This is an extremely costly process and there have been instances where stents have been shelved at a late stage of development due to poor results. There is a growing recognition within the community that a truly multi-disciplinary approach is required to design the next generation stents, with mathematical and computational modelling playing a key role. Indeed, ideas from several branches of mathematics are required to successfully tackle this problem. Currently, a number of approaches are being adopted, including methods from continuum mechanics and mathematical biology, inverse problem theory, structural and soft tissue mechanics, numerical analysis and multi-objective optimisation. In modelling drug transport, which is the focus of this talk, analytical/semi-analytical and asymptotic approaches to solving coupled systems of advection-diffusion-reaction equations have been considered, moving boundary problems have been defined, and finite difference/finite element methods have been devised to cope with increasing complexity. But the scope is far wider: for example, agent based models and machine learning approaches may well find application here.

The purpose of this talk is two-fold. Firstly, it aims to provide a flavour of the purpose and evolution of stents and the modelling approaches that have been adopted thus far [1]. Secondly, a case study will be presented from our own group, which demonstrates how mathematical modelling has influenced the design of a novel drug-eluting stent [2].

Keywords: Stents, drug release, advection-diffusion-reaction, fluid dynamics.
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Optimizing the performance of drug-eluting stents: simulations and experiments

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Despite the undisputed success of drug-eluting stents (DES), there is a persistent risk of serious complications including in-stent restenosis, late stent thrombosis, and stent fracture. Mechanical stresses within the arterial wall induced by stent implantation contribute to the incidence of restenosis [1,2]; therefore, it is desirable to target stent designs that minimize these stresses. DES thrombosis is primarily attributable to delayed endothelialization because the drugs used in DES inhibit endothelial cell proliferation and migration [3]; thus, there is a need for designing appropriate DES drug release strategies that minimize drug concentration at the endothelium. Finally, the likelihood of occurrence of DES fracture increases with the push towards thinner stent struts that reduce arterial wall injury upon stent deployment and perturb the flow field minimally. In light of the above, DES design involves a myriad of competing considerations and hence calls for multi-variable optimization. The goal of the present study is to optimize DES strut dimensions and drug release dynamics so as to meet the following set of specific objectives: 1) deliver efficacious but sub-toxic drug loads to the arterial wall in order to effectively control restenosis, 2) have minimal drug concentration at the endothelial surface in order to allow rapid stent endothelialization, 3) disturb the flow field minimally, 4) provide mechanically stable stent struts to avoid fracture given the loads to which the stent is subjected, and 5) induce minimal stresses in the arterial wall. A multi-physics computational model is developed that describes drug release from DES, drug convective and diffusive transport as well as drug reaction within the arterial wall, mechanical stresses within both the stent and a hyperelastic arterial wall, and the flow field within the arterial lumen. The model is subsequently used to optimize stent strut dimensions and drug release dynamics in order to meet the objectives described above. The optimization is performed using a gradient-free approach based on the surrogate management framework. The optimization results demonstrate that drug release dynamics depend strongly on the type of drug used and that optimal strut dimensions need to strike a balance between the effect on lumenal blood flow and on transmural stresses. In order to be able to experimentally test the predictions of the DES optimization studies, we have developed an in vitro coronary artery model which consists of an annular collagen hydrogel within which smooth muscle cells are embedded and whose lumenal surface is lined with endothelial cells. Endothelial wound healing as well as smooth muscle cell migration after stenting are monitored and quantified in the in vitro artery. Moreover, particle image velocimetry is used to measure the flow field within this artificial artery and to quantify the wall shear stress both within and outside the stented zone.

Keywords: stents, optimization, drug release, mechanical stresses, flow disturbance.
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Mathematical models of drug release from polymer-free drug-eluting stents

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Polymer-free drug-eluting stents are an innovative new treatment for coronary heart disease which is the leading cause of death globally. In these polymer-free stents, the drug is either sprayed directly onto a bare metal surface or infused in a metallic porous medium. They have the potential to overcome problems associated with the current best treatment: polymer-coated drug-eluting stents. However with no polymer to control drug release, it is unclear how desired release rates can be achieved. In this talk, the first model of drug elution from polymer-free stents is presented. The generalised model is capable of predicting the drug release from a number of polymer-free systems including those that exhibit nanoporous, nanotubular and smooth surfaces. The model is based principally on dissolution theory and the theory of diffusion in porous media. Analytical solutions are derived to determine the important parameters that control the release rate. Drug release profiles are also provided, and design recommendations are offered so that the release profile may be tailored to achieve the desired outcome. Note that the models presented here are for drug release in an in-vitro environment. These models are not specific to drug-eluting stents and may also be applied to other biomedical implants that use nanoporous surfaces to release a drug.

Keywords: Polymer-free stents, mathematical model, dissolution, diffusion, drug release, nanoporous materials.

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Variable porosity coatings as a means of controlling drug release from stents

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Much of the research concerned with drug-eluting stents is focussed on developing sophisticated computational models which accurately simulate drug release and tissue absorption. The complexity of these models is increasing, with more and more realistic features being accounted for, including accurate 3D geometrical representations of the stent and multi-layered artery, anisotropic and spatially-varying tissue properties and multiple drug binding reactions. If, on the one hand, these models are indeed necessary to accurately simulate drug transport in the biological tissue, on the other hand it is clear that stent manufacturers cannot intervene on the underlying biology. What they can control, however, are the properties of the stent platform and the coating. Therefore, in this talk, we take a step back from the fully coupled computational models (see e.g. [1, 2]) and focus instead solely on the properties of the stent coating.

The drug is typically contained within some durable/biodegradable polymer coating or embedded within a nanoporous structure. The drug release profile depends on a number of factors including the porosity of the coating or bulk structure; the drug loading and initial distribution; the physico-chemical properties of the drug (e.g. molecule size, solubility, etc.), and the release medium. A certain level of control is required, for example an excessive amount of drug delivered too quickly can result in toxicity whilst too little drug will have no therapeutic effect. However, the most desirable release profile may be patient-specific and is in fact the subject of some controversy.

In this work we propose variable porosity as means of controlling the drug release and tailoring the drug release profile. Focussing initially on drugs that are contained within a porous polymer coating, we develop a mathematical model for the drug transport accounting for both spatially and temporally varying porosity [3]. The former could be either a smoothly varying porosity throughout the coating, or a layered structure, with each layer encompassing a different level of porosity. The porosity may also vary with time as a result of dissolution, degradation, erosion or fluid ingress [4]. The results may be useful in the coating manufacture to assess an optimal control strategy for the rational design of tomorrow's advanced drug-eluting systems.

Keywords: Drug release, porous media, mathematical modelling.
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Numerical simulation of drug transport in arterial wall under healthy and atherosclerotic conditions

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The objective of this contribution is to propose a numerical model of drug transport in the arterial wall for healthy and pathological conditions. Atherosclerosis is the process in which deposits of fatty substances, cholesterol, cellular waste products, calcium and other substances are built in the inner lining of an artery. These deposits are called plaques. Drug-eluting stents (DES) have become the most successful device to deal with advance atherosclerotic lesions. DES are metal devices that have been coated with a pharmacologic agent (drug) that is known to suppress restenosis: the reblocking or closing up of an artery after angioplasty due to excess tissue growth (SMCs proliferation and migration) inside or at the edge of the stent. The development of DES has effectively caused almost completely detention of wall restenosis. However these antipoliferative drugs can slow down the healing process on the endothelium that should follow to stent implantation. This healing delay is related with an elevated risk of late vascular thrombosis. The purpose of these devices is to release the specific drug concentration to inhibit SMCs proliferation appearing during first stages after angioplasty but avoiding toxicity interaction that can affect to arterial wall integrity.

A numerical model of drug transport in the arterial wall for healthy and pathological conditions is presented in this work. The artery is described as an axi-symmetric five-layer model including lumen, endothelium, subendothelial space, internal elastic lamina and media following previous literature models [1]. In the arterial lumen domain, the blood flow simulation is based on incompressible Navier-Stokes equations. The arterial wall is considered as a heterogeneous porous medium. Darcy's law is employed to describe the transmural flow and the filtration velocities through porous layers are calculated applying it. Convection-diffusion equation is taken into account to model the transport of drug in flowing blood while convection-diffusion-reaction processes are used to model drug transport through subendothelial space and media. The flux across endothelium and internal elastic lamina is described using the Kedem-Katchalsky equations. Also, a saturable reversible binding model is incorporated to describe the interaction between drug and smooth muscular cells of the arterial wall. The transport parameters of this model are obtained from literature and some of them are fitted to describe experimental evidences, including equilibrium tissue incubation and endovascular and perivascular drug application [2]. Two of the most used antiproliferative drugs are studied and compared, paclitaxel and sirolimus. The transport and binding features of both drugs are studied under different wall situations, considering healthy conditions for the artery and under the presence of an atherosclerotic plaque. Finally, distinct conditions for the drug release, such as type of release device, drug dose or exposition time, are also analyzed.

Keywords: drug diffusion, drug deposition, arterial wall, convection-diffusion-reaction equation.
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MS03: Moving boundary problems in industrial applications

MS03: Moving boundary problems in industrial applications

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Moving boundary problems appear in the modelling of a variety of physical processes including phase-change (melting and solidification), the dissolution of a solid in a solvent and fluid dynamics. Due to this broad scope, we see moving boundary problems in many industrial applications including (but not limited to) metal-casting, nanotechnology and pharmacology. Here we present a collection of studies from these diverse fields and we highlight various analytical and numerical techniques.

The problems presented here are perfect examples of applying mathematical models to industrial applications. Such endeavours promote cooporation between mathematicians and industry and contributes to the core principals of ECMI.

Speakers:

F. Font. MACSI. *Influence of substrate melting on the laser-induced dewetting of nanothin films.*

S. Mitchell. MACSI. *The effect of superheat on the macrosegregation of a continuously cast binary alloy.*

K. Devine. MACSI. *Mathematical modelling of the formation of oscillation marks in the continuous casting of steel.*

B. J. Florio. MACSI. *Mathematical modelling of phase change in nanowires.*

V. Cregan. Centre de Recerca Matemàtica, Barcelona. *Nanoparticle growth via the precipitation method*.

N. McInerney. MACSI. *A moving boundary problem in controlled release pharmaceuticals.*

Keywords: Moving boundary problems; Phase change; Industrial modelling.

Influence of substrate melting on the laser-induced dewetting of nanothin films

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Dewetting of thin nanoscale metallic films has shown promise as a self-assembly process for synthesizing large-area correlated nanoparticle ensembles [1, 2]. This process involves laser irradiating a metal nanothin film sitting on a substrate with lower thermal conductivity. After laser irradiation, the temperature of the metal, initially in a solid state, raises over the melting point and the metal becomes a liquid. The thin liquid layer is unstable and so breaks up into droplets. In the absence of further heating the droplets subsequently solidify. Experimental observations suggest that the high temperatures reached during laser irradiation lead to partial melting of the substrate, which presumably affects the dewetting behavior of the metal film. In this talk, I will present a one-dimensional model describing the heat transfer and phase change of the metal/substrate set up after laser irradiation and discuss the possible effects of a molten substrate in the dewetting process.

Keywords: Laser heating, melting, nanothin films.
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The effect of superheat on the macrosegregation of a continuously cast binary alloy

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Keywords: macrosegregation; continuous casting; alloys; boundary immobilization

Macrosegregation, i.e. the lack of homogeneity of the solute concentration at the whole scale of a solidified product, is a central problem in the continuous casting of metal alloys, since it strongly influences the further workability of the cast products and their mechanical properties. As already established by Flemings and co-workers [1, 2], macrosegregation is the result of slow interdendritic flow of molten liquid and the transport of alloying elements at the product scale.

Mathematically, the problem involves coupled momentum, heat and mass transfer in a translating, solidifying porous medium. Although the problem is often tackled using techniques of computational fluid dynamics (CFD), here we continue the development of an asymptotics-based approach that makes use of the fact that interdendritic flow is predominantly driven by solidification shrinkage [3], which can be expressed in terms of a small dimensionless parameter, $\rho_s/\rho_l - 1$, where ρ_s and ρ_l are the solid and liquid phase densities, respectively. Whereas earlier work developed the framework for the case of zero superheat, i.e. where the casting temperature, T_{cast}, is equal to the liquidus temperature, T_{liq}, here we include the effect of superheat, so that $T_{cast} > T_{liq}$. This gives rise to a further small dimensionless parameter, which allows for significant simplification of the governing system of equations which are then solved hierarchically.

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Mathematical modelling of the formation of oscillation marks in the continuous casting of steel

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Continuous casting has been developed industrially worldwide since the 1950s as a high-throughput method for producing, amongst other things, metal billets, blooms and slabs; more than 90% of the world's steel is produced this way, amounting globally to more than one billion tonnes of steel cast per year. During casting, liquid steel is poured into the top of a water-cooled copper mould, where intense cooling causes a solidified steel shell to form. To prevent the steel sticking to the mould wall, a flux powder is added to the surface of the steel and the mould is oscillated at high frequency; the process is further complicated by low frequency phenomena associated with the turbulent flow of molten steel and the meniscus level fluctuations. All of these combine to produce undesired imperfections on the steel surface, which are expensive to remove, and a process that is both difficult to predict and control.

In order to formulate our model we refer to the work by Hill et al. [1, 2] which is more amenable than some numerical models [3, 4, 5, 6]. We use a lubrication approximation in the liquid flux region. Heat flow in the steel and flux is considered and coupled with the flow equations to predict mark formation. The model is non-dimensionalised in a systematic way. By neglecting small terms we obtain a model which makes fewer a priori assumptions than in [2]. We then proceed with our analysis by relaxing some dimensionless parameters and a qualitative result is obtained.

Keywords: Continuous Casting, Stefan Problems, Asymptotic Analysis, Moving Boundary, Industrial Mathematics
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Mathematical modelling of phase change in nanowires

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Recent research indicates that in the near future nanowires will be at the forefront of electronics and computing. It has also been shown that they can be utilised in low cost solar cells, high power density batteries, flexible screens, to detect proteins to act as cancer biomarkers and for water filtration [1, 2, 3, 4]. One feature observed in nanoparticles is the depression of the melting point from the bulk value. For example, 1 nm radius gold particles show a decrease of 50% from the bulk melting value [5]. This has implications in nanoelectronics where the load-carrying capacity of nanowires may be limited by the melting point depression.

We use continuum theory to model the melting behaviour of cylindrically symmetric nanowires in a thermal bath. The melting point depression is described by the Gibbs-Thomson equation. This continuum approximation is valid down to approximately 2 nm [6]. The problem is treated semi-analytically by a perturbation expansion in the large Stefan number. The results are compared with similar approaches for spherical nanoparticles. An equivalent solidification problem is also studied.

We found that the melting of a nanowire occurs much slower than the melting of a nanosphere with same radius. This is due to fewer degrees of freedom and the smaller effect of the melting point depression in the cylindrical geometry. The melting and solidification processes are shown to be different due to the release of surface energy from the solid-liquid interface as it decreases in size.

Keywords: Nanowire; Melting point depression; Stefan problem.
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Nanoparticle growth via the precipitation method

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Nanoparticles are small units of matter with dimensions in the range 1-100 nmthat lie at the interface of bulk materials and atomic structures. Whilst the physical and chemical properties of bulk materials tend to be independent of size, at the nanoscale, size strongly dictates material properties. Consequently, nanoparticles exhibit many advantageous size-dependent magnetic, electrical, chemical and optical properties. These properties are extremely sensitive to the particle size, and thus the ability to produce monodisperse particles that lie within a controlled size distribution is critical.

Due to its ease of use, precipitation of nanoparticles from solution is currently one of the most widely employed synthesis methods [1, 2]. Typically, the nucleation and growth processes are separated, where the former is used to generate seeds for the latter. The resulting two-phase system is not in its lowest possible energy state due to the presence of small particles. Thermodynamic equilibrium is achieved by Ostwald ripening, whereby large particles grow at the expense of the more soluble small particles. This leads to the unwanted defocusing of the particle size distribution (PSD), caused by growth and dissolution of bigger and smaller particles, respectively. The PSD can be refocused by changing the reaction kinetics by the addition of precipitating material, or varying the temperature or pH [4, 5]. However, the main disadvantage of this process is that the precise relationship between particle growth and system conditions is still not fully understood [3].

We consider the evolution of a system of nanoparticles in solution via size focusing and Ostwald ripening. The model consists of a diffusion equation for the concentration of the solution, Stefan-type conditions to track the particle-liquid interfaces and a time-dependent expression for the bulk concentration obtained via mass conservation. Rescaling the model leads to a small, dimensionless parameter in front of the time derivative term in the diffusion equation, which is the basis of a pseudo-steady state solution for the concentration. This solution is substituted into the Stefan conditions to yield a system of ordinary differential equations for the particle radii. The model is solved numerically to give the evolving PSD from which we measure the average particle radius and standard deviation. The results are shown to be in good agreement with experimental data for cadmium selenide nanoparticles [5].

Keywords: Nanoparticle; monodispersity; size focusing; Ostwald ripening; liquid-phase synthesis; diffusion equation; Stefan condition.
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A moving boundary problem in controlled release pharmaceuticals

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Polymer based controlled drug delivery devices are becoming increasingly popular in the pharmaceutical industry, due to the ability of chemists to synthesise polymers with desired properties to suit a required release profile. This can alleviate the disadvantages of traditional drug delivery, such as inaccurate dosages and patient compliance, minimising toxicity and maximising effectiveness. Mathematical modelling is an important tool in facilitating product development in the pharmaceutical industry, assisting is determining the geometries and configurations of these devices, as well as the desired drug loading concentrations.

Whilst there has been extensive studies of drug release mechanisms both from a theoretical and experimental point of view, there is little research into fully understanding the moving interface between the dissolved and loaded drug, especially in the case of swelling polymers where the polymer changes from a fully swollen to a fully collapsed state upon contact with an environmental fluid. In swelling controlled devices the polymer matrix is initially in a dry glassy state with the drug molecules dispersed and unable to diffuse. The polymer swells upon contact with an environmental fluid (solvent), which then diffuses into the polymer (often hydrophilic hydrogels), creating a moving boundary separating the dry polymer from the now swollen rubbery polymer, within which the drug can now diffuse. There is also a second moving boundary at the edge of the polymer as a result of volume change.

We revisit the work of Cohen and Erneux [2], who proposed a coupling of the popular Higuchi [3] model describing drug release with the Astarita and Sarti [1] model describing a solvent penetrating a polymer in one dimension. This Stefan problem then has two distinct sections, the first describes the concentration of the solvent $C(X,T)$ that diffuses into the device and the position of the two moving boundaries $S_1(T)$ moving into the polymer and $S_2(T)$ moving outwards because of the volume change. The solutions for $S_1(T)$ and $S_2(T)$ are then used as an input into the second section of the model describing the countercurrent diffusion of the drug with concentration $A(X,T)$.

We suggest a different scaling to Cohen and Erneux, recovering three non-dimensional parameters in the process, all of whose size can vary. We then extend their analysis by doing small and large time asymptotics, but these are limited due to the parameter sizes needing to be $O(1)$. We then apply the popular heat balance integral method (HBIM) and refined integral method (RIM), and describe how to optimise the exponents of the approximating polynomials for both the solvent and drug. The results are shown to be accurate for all time and varied parameter values.

Keywords: Controlled drug release, Stefan problem, drug diffusion, solvent penetration, asymptotics, heat balance integral method.

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MS04: Return of experience from Study Groups

MS04: Return of experience from Study Groups

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Study Groups with Industry are now a well established tool throughout Europe (and beyond) to promote industrial mathematics. This MS will give the opportunity to PhD students who have recently participated in such Study Groups to report on their experience, present results obtained during the Study Group, and indicate the follow up of their work. This MS will also show the diversity of topics and applications addressed in Study Groups. It will give visibility to the PhD students and advertise about Study Groups towards all public (students, faculty and industrialists) attending the ECMI conference.

The MS will feature the following talks :

M. Kresoja, S. Rackov. University of Novi Sad. *Modelling Credit Scorecard with Time-Dependent Variables.*
In order to meet regulatory requirement in the most efficient manner, all major banks are using Internal Rating Based (IRB) approach. As a result, expected loss that banks are exposed to, can be minimized and available funds for further investments can be increased, which all leads to profit maximization. Good credit risk management under the IRB approach includes optimization and development of three main risk drivers: probability of default (PD), exposure at default (EAD) and loss given default (LGD). In this research we will focus on modelling the probability of default of a borrower and propose two approaches: survival analysis and machine learning algorithms.
Using real data set provided by one Serbian bank, we have implemented proposed solutions and compared it with the classical logistic regression. The overall results showed that both approaches outperform the logistic regression. Method with the most superior performance was Support Vector Machine. The performances of the models were evaluated by Gini coefficient and KS statistics. Time dependent variables with highest discriminatory power were inflation index and exchange rate.

C. Courtès, G. Dusson, R. Hatchi, R. Molina, A. Thomas. University Paris XI (France). *Compressed sensing applied to radar imaging.*
For aircraft industry in which Airbus Group evolves, identifying features of a plane or of an helicopter which is flying over a given area is a crucial point. Those features are mathematically modelled by a sparse function g with only a few dominant point-like scattering centers localized on strategic positions of the airplane. In practice, companies do not have access to the sparse function but only to measurements made by radars. An important issue is then to reconstruct satisfactory signal from those measurements.
The compressed sensing is based on two steps : acquisition of directly compressed data and a nonlinear reconstruction. The first stage consists in obtaining random measurements (not matching initial signal structure at all), while the second phase performs the sparse recovery via a convex l1-minimization. Applying this algorithm to the radar imaging processing is the aim of this talk.

M. Cruz, I. C. Lopes, A. Mota e Silva. Polytecnic of Porto (Portugal). *Packing and shipping cardboard tubes.*
SpiralPack - Manipulados de Papel, S.A. is a Portuguese company specializing in the production of tubes, angles, multipurpose packaging and cardboard formwork, which supplies their products to several sectors and is one of the main Iberian peninsula players in the production of standard and high performance cardboard tubes. In the context of tube manufacturing, there are certain processes that SpiralPack would like to improve. With a production totalling almost 17.5 million tubes/year, arising from more than 1500 different specifications corresponding to almost 100 tubes with different diameters, an

important part of Spiralpack resources is allocated to packing and shipping processes. The company attended to the 101st European Study Groups with Industry (ESGI), held in Faculdade de Ciencias da Universidade Nova de Lisboa to address the following questions: (1) Given an order for a certain tube specification possibly with a grouping request, what is the maximum number of tubes that can be packed inside a given container (usually the truck space) and how should they be positioned? (2) Given several pallets of tubes, what is the most efficient way to arrange them in a container? (3) Are there more efficient ways to group and pack tubes than the ones currently used? In this talk, we will address briefly the options, research and developments made during and after the 5-day 101st ESGI.

A. Levitt. University Paris Dauphine (France). *SEME 2015: Trajectory optimization for bathymetric navigation.*

This study group project took place in January 2015, and involved six PhD students and postdocs. The subject, provided by iXBlue, was bathymetric navigation. A submarine can measure its elevation with respect to the seafloor, and compare it to known maps to improve its localization. The question submitted to us was to find paths that allowed for a good positioning of the submarine in this way.

We investigated a number of different formalizations of this problem (a graph modelization, a probabilistic approach, and a formulation as an optimal transport problem), and proposed a solution that yielded a non-trivial but plausible behaviour (follow the ridges of the map).

Modelling credit scorecard with time-dependent variables

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In order to meet regulatory requirement in the most efficient manner, all major banks are using Internal Rating Based (IRB) approach. As a result, expected loss that banks are exposed to, can be minimized and available funds for further investments can be increased, which all leads to profit maximization. Good credit risk management under the IRB approach includes optimization and development of three main risk drivers: probability of default (PD), exposure at default (EAD) and loss given default (LGD). In this research we will focus on modelling the probability of default of a borrower and propose two approaches: survival analysis and machine learning algorithms. In practice, the most common approach for estimating probability of default is binary logistic regression [1]. Using logistic regression, probability that borrower will default is predicted within the fixed time period, usually time window of one year is taken. The dependent variable takes value one if a borrower has defaulted in the observation period and zero otherwise. The set of independent variables consists of all relevant variables from the borrower's credit bureau and application forms. Significant independent variables are selected via stepwise method. Although being industry standard, logistic regression cannot model borrower's status during the actual loan repayment period if the maturity of a loan is long term. Moreover, this approach cannot easily include impact of dynamic conditions on borrower's reimbursement capacity. General conditions in the economy like exchange rate change, inflation rate, interest rate, consumers basket can have important influence on credit risk [2]. In order to overcome the shortcomings and to improve the current practice, we have first implemented Cox PH proportional hazards regression with time-dependent covariates [3]. In certain way, it can be thought as extension of logistic regression that allows to model not just if a borrower will default, but also the time when default status occurs. Proposed method allows incorporating macroeconomic environment and examining which macroeconomic factors have influence on probability of default. To improve the variable selection process, Lasso method is used as regularization procedure instead of stepwise selection [4]. As a second approach for probability of default model development, Support Vector Machine is implemented [5]. It is artificial learning technique used in binary classification which relies on the linearity in a high-dimensional space and on the optimization. Using real data set provided by one Serbian bank, we have implemented proposed solutions and compared it with the classical logistic regression. The overall results showed that both approaches outperform the logistic regression. Method with the most superior performance was Support Vector Machine. The performances of the models were evaluated by Gini coefficient and KS statistics. Time dependent variables with highest discriminatory power were inflation index and exchange rate.

Keywords: probability of default, time dependent variables, Cox PH model, Lasso method, support vector machine.

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Compressed sensing applied to radar imaging

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For aircraft industry in which Airbus Group evolves, identifying features of a plane or of an helicopter which is flying over a given area is a crucial point. Those features are mathematically modelled by a sparse function g with only a few dominant point-like scattering centers localized on strategic positions of the airplane. In practice, companies do not have access to the sparse function g but only to measurements made by radars. An important issue is then to reconstruct satisfactory signal $\widehat{g}$ from those measurements.

Conventionally, the Fourier inverse transform is used and the original signal is perfectly reconstructed provided two conditions are met : uniform samples and sampling frequency at least twice the Fourier bandwith (according to the so-called Shannon-Nyquist theorem). However, a method developed as part of signal processing could be used to reduce drastically the required measurements and to get away from dependence of the initial signal : the compressed sensing.

The compressed sensing [1, 3] is based on two steps : acquisition of directly compressed data and a nonlinear reconstruction. The first stage consists in obtaining random measurements (not matching initial signal structure at all), while the second phase performs the sparse recovery *via* a convex ℓ^1 minimization. Applying this algorithm to the radar imaging processing is the aim of this talk.

This work [2], conducted in close collaboration with Airbus Group, is one of the projects suggested in the 12$^{\text{th}}$ SEME which took place in Paris in January 2015. The SEME (Semaines d'Etude Maths-Entreprise) are very much in line with the European Study Groups in Industry, initiated in England in the 1960s. This french equivalent supported by the Labex AMIES aims to strengthen the partnerships between the academic community and industry.

Keywords: Compressed sensing, inverse problem, radar imaging, signal processing
Acknowledgments. The 12$^{\text{th}}$ SEME was supported by the french Labex AMIES, together with the laboratory LJLL (UPMC and Univ. Paris Diderot) and the laboratory LAGA (Univ. Paris 13).

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Packing and shipping cardboard tubes

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SpiralPack - Manipulados de Papel, S.A. is a Portuguese company specializing in the production of tubes, angles, multipurpose packaging and cardboard formwork, which supplies their products to several sectors and is one of the main Iberian peninsula players in the production of standard and high performance cardboard tubes. In the context of tube manufacturing, there are certain processes that SpiralPack would like to improve. With a production totalling almost 17.5 million tubes/year, arising from more than 1500 different specifications corresponding to almost 100 tubes with different diameters, an important part of Spiralpack resources is allocated to packing and shipping processes.

The company attended to the 101^{st} European Study Groups with Industry (ESGI), held in Faculdade de Ciências da Universidade Nova de Lisboa to address the following questions:

(1) Given an order for a certain tube specification possibly with a grouping request, what is the maximum number of tubes that can be packed inside a given container (usually the truck space) and how should they be positioned?
(2) Given several pallets of tubes, what is the most efficient way to arrange them in a container?
(3) Are there more efficient ways to group and pack tubes than the ones currently used?

In this talk, we will address briefly the options, research and developments made during and after the 5-day 101^{st} ESGI that lead to the following achievements:

- It is not possible to have an heuristic that achieves the most efficient package layout without using a mathematical model and so, most probably Spiralpack is not efficient with a packing system based on employees intelligence.
- A tailored mathematical model was developed to address this problem in order to be human-feasible, that is, we consider only tube orientations that may be accomplished manually.
- With the developed model, given a certain demand, it is possible to calculate the maximum number of tubes that can be shipped inside the container and to know how many pallets of different sizes and configurations should be used in order to minimize the total volume or area.
- Since the problem of arranging pallets of tubes in a container is NP-hard, and the Spiralpack hardware and software resources are limited, an heuristic was proposed to tackle this problem.
- After several tests on-site, the model was tuned to fit other constrains important to the company daily operations (e.g. how the tubes are tied together into sets that can be handled by workers)
- In order to help Spiralpack tackle their initial problem, a software package was produced that fully integrates with their information system.

Keywords: Circle packing, Container loading, European Study Groups with Industry, ESGI, Mathematics in Industry, Mathematical Modelling

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SEME 2015: Trajectory optimization for bathymetric navigation

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SEME (Semaine Mathématiques Entreprises) are week-long study groups. This project took place in January 2015, and involved six PhD students and postdocs. The subject, provided by iXBlue, was bathymetric navigation. A submarine can measure its elevation with respect to the seafloor, and compare it to known maps to improve its localization. The question submitted to us was to find paths that allowed for a good positioning of the submarine in this way.

We investigated a number of different formalizations of this problem (a graph modelization, a probabilistic approach, and a formulation as an optimal transport problem), and proposed a solution that yielded a non-trivial but plausible behaviour (follow the ridges of the map).

MS05: Fluid instabilities and transport phenomena in industrial processes

MS05: Fluid instabilities and transport phenomena in industrial processes

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This mini-symposium will focus on the mathematical modeling and analysis of processes occurring in industry (for example, food and drink, pharmaceutical, and oil sector). These are some of the challenging industrial problems currently under investigation at the Mathematics Application Consortium for Science and Industry (MACSI) in Ireland. The talks will cover the development of innovative mathematical models that are intended to help industry optimize and improve processes. Models are devised for mass transfer in particulate systems, e.g. solid-liquid extraction, particle-laden viscous flows, and stability/instability problems in liquid bridges and two-phase flows. Asymptotic, analytical, and numerical techniques are used to investigate the solutions of the proposed mathematical models.

Speakers:

K. Moroney. MACSI, University of Limerick (Ireland). *Asymptotic analysis of a coffee extraction model for a fixed coffee bed.*

M. Haynes. MACSI, University of Limerick (Ireland). *Equivalence of stability methods for a horizontal liquid bridge.*

R. Barros. MACSI, University of Limerick (Ireland). *Particle-laden viscous suspensions in an inclined channel.*

S. Kaar. MACSI, University of Limerick (Ireland). *Separation of bubbles in Guinness leading to instability waves.*

W. Arne. Fraunhofer ITWM (Germany). *Viscoelastic law for Cosserat rod models with application in rotational spinning processes.*

J. Duley. MACSI, University of Limerick (Ireland). *A model for heterogeneous nucleation and short term growth of molecular clusters.*

Keywords: Mathematical modelling, Nucleation, Crystallisation, Solid-liquid extraction, Asymptotic analysis, Fluid dynamics, Viscous flows, Linear Stability, Particle-laden flows, Visco-elastic flows.

Asymptotic analysis of a coffee extraction model for a fixed coffee bed

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The extraction of soluble coffee from a porous bed of roast and ground coffee grains is a complex process. The properties of the resulting dilute solution of extracted coffee solubles and hot water depend on a large number of brewing parameters. Achieving accurate and repeatable extraction of coffee solubles is a key challenge to consistently brewing high quality coffee.

Here we consider a recently published, experimentally validated model of coffee extraction [1]. Extraction of coffee is described using a double porosity model, which includes the dissolution and transport of coffee. It is shown that the model can describe extraction curves from experiments in two situations: extraction from a dilute suspension of coffee grains and water, and extraction from a packed coffee bed. Previously, the motivation and derivation of this model via volume averaging was the subject of a contributed talk at ECMI 2014. In this study we consider asymptotic solutions to the model of coffee extraction in a packed bed.

At the scale of the coffee grain, extraction is modelled by two processes. Rapid dissolution of coffee from the broken cells on the grain surface dominates extaction initially. As coffee near the grain surface is depleted, extraction from the grain kernel begins to dominate. The grain kernel consists of a network of intact coffee cells. The much slower diffusion of coffee through the intragranular pore network to the grain surfaces, drives extraction for the rest of the brewing time. Extraction of coffee is also dependent on the speed of advection of coffee from the bed. To obtain asymptotic solutions for the coffee concentrations in and exiting the bed, we utilise the small parameter resulting from the ratio of the advection timescale to the grain diffusion timescale. The resulting initial layer and outer solutions are matched using the method of matched asymptotic expansions. The asymptotic solutions are compared with the numerical solutions of the model and available experimental data.

Keywords: Double porosity model, Coffee brewing process, Coffee extraction kinetics, Solid-liquid extraction, Asymptotic analysis, Matched asymptotic expansions.
Acknowledgments. The authors acknowledge the support of MACSI, the Mathematics Applications Consortium for Science and Industry (www.macsi.ul.ie), funded by the Science Foundation Ireland Investigator Award 12/IA/1683.

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Equivalence of stability methods for a horizontal liquid bridge

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We consider a liquid bridge held inside a cylinder. In this geometry equations for the shape of the bridge are found, first by using variational techniques on the free energy of the system and then showing this gives the same equations as the use of the Navier-Stokes equations.

By then considering the second variation of the free energy while in this static case derive an eigenvalue problem to determine the stability of this static case. A similar eigenvalue problem is derived using linear stability methods on the Navier-Stokes equations. We then show that these eigenvalue problems are equivalent.

Keywords: Fluid Instabilities, Young-Laplace Equation, Variational Methods, Navier-Stokes equations, Linear Stability

Acknowledgments. We acknowledge the support of the Mathematics Applications Consortium for Science and Industry (www.macsi.ul.ie) funded by the Science Foundation Ireland grant investigator award 12/IA/1683.

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Particle-laden viscous suspensions in an inclined channel

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We characterize the flow of a viscous suspension in an inclined channel where the flow is maintained in a steady state under the competing influences of gravity and an applied pressure drop. The basic model relies on a diffusive-flux formalism. Such models are common in the literature, yet many of them possess an unphysical singularity at the channel centreline where the shear rate vanishes. We therefore present a regularization of the basic diffusive-flux model that removes this singularity. This introduces an explicit (physical) dependence on the particle size into the model equations. This approach enables us to carry out a detailed parameter study showing in particular the opposing effects of the pressure drop and gravity. Conditions for counter-current flow and complete flow reversal are obtained from numerical solutions of the model equations. These are supplemented by an analytic lower bound on the ratio of the gravitational force to the applied pressure drop necessary to bring about complete flow reversal.

Keywords: Particle-laden viscous flow, Diffusive-flux model, Regularized model, Inclined channel.
Acknowledgments. The authors acknowledge the support of MACSI, the Mathematics Applications Consortium for Science and Industry (www.macsi.ul.ie), funded by the Science Foundation Ireland Investigator Award 12/IA/1683.

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Separation of bubbles in guinness leading to instability waves

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Separation processes are important in the chemical engineering of food, drink and pharmaceuticals. The settling of a freshly poured pint of stout beer provides an observable example of bubble separation. Bubbles appear as a white cloud against the black beer. A strange phenomenon is that the bubbles appears to descend in waves at the glass. The mechanism of these waves has been modelled as an instability leading to roll waves by Robinson *et al.* [1]. This model assumed the existence of sinking bubbles. Benilov *et al.* [2] explained the origin of the sinking bubbles by a simple physical mechanism and confirmed their results by CFD simulation. However, their simulations did not show wave formation. A framework which explains both sinking bubbles and the resulting waves is studied here. We show that in a typical glass of beer there is a circulation: the beer rises, except for a narrow band at the perimeter where it descends. The width of this faster downward flow is related to the rising bubbles and their simultaneous motion away from the side of the glass. This flow has a radial velocity profile across the glass with the correct viscous shear flow characteristics necessary to generate flow instability and therefore observable waves.

Keywords: Two phase, Seperation processes, Instability waves.
Acknowledgments. The authors acknowledge the support of MACSI, the Mathematics Applications Consortium for Science and Industry (www.macsi.ul.ie), funded by the Science Foundation Ireland Investigator Award 12/IA/1683.

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Viscoelastic law for Cosserat rod models with application in rotational spinning processes

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The rotational spinning of viscous jets is of interest in many industrial applications, including drawing, tapering and spinning of glass and polymer fibers. In rotational spinning processes, hot liquid jets leave the small spinning nozzles located on the curved face of cylindrical disc that rotates about its symmetry axis. The extruded jets are stretched and cooled by the surrounding air flow to become the fibers thin and hardened. To simulate such a process we use Cosserat rod models [1] to describe the fiber dynamics and three-dimensional Navier-Stokes equations for the air flow. Both are combined in an iterative two way coupling concept [2]. The fibers are cooled very fast and the simulation with a viscous law is restricted to short fibers. The viscoelastic UCM-type law for an one-dimensional string model is developed in [4], for general overview in 3D we refer to [3]. Our new developped viscoelastic material law for the Cosserat rod model overcomes this restriction and allows simulation of longer fibers with realistic behavior in the air. The UCM-type law shows the viscous limit [5] if the relaxation time goes to zero and on the other side it has an elastic limit [1] if the viscosity goes to infinity. Simulation results are shown for the example of a centrifugal rotational spinning process [2] of the polymer fibers.

Keywords: Cosserat rod, viscoelastic, two way coupling, rotational spinning process
Acknowledgments. This work has been supported by German DFG, project 251706852, MA 4526/2-1, WE 2003/4-1.

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A model for heterogeneous nucleation and short term growth of molecular clusters.

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In the context of the precipitation of solid crystals from a supersaturated solution, we develop a model for heterogeneous nucleation of these crystals onto an impurity with a view to exploring time scales for the process.

Numerical experiments are conducted considering molecular adsorption and dissolution as a stochastic process. Each experiment ultimately generates a profile for cluster size distribution averaged via Monte-Carlo methods. In parallel to these experiments discrete difference equations are derived to model the expected behaviour of the above mechanism. A continuum hypothesis is then invoked to result in a non-local, non-linear PDE for which numerical solutions are found and ambitions for asymptotic solution held.

Keywords: Nucleation, Crystallisation, Random sequential adsorption [RSA], Population Models.
Acknowledgments. This research is generously supported by a grant from Science Foundation Ireland [SFI] through the Mathematics Applications Consortium for Science and Industry [MACSI] group at the University of Limerick.

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MS06: Advanced numerical methods for hyperbolic problems

MS06: Advanced numerical methods for hyperbolic problems

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The purpose of the mini symposium is to gather researches interested in industrial application of numerical methods for hyperbolic problems. Hyperbolic systems are involved in the description of many physical problems, ranging from classical applications in aerodynamics to shallow water models for the simulation of waves in lakes and rivers, from combustion problems to hydrodynamical models of semiconductors, to mention just a few examples. Because of the actuality and impact of the subject, a recent European Marie Curie ITN project, called ModCompShock (Modelization and computation of shocks and interfaces) has been approved and has just started. The project involves eight main European Universities and several partner research centers. Several participants to the project will be invited to contribute to the mini symposium, which will become a unique opportunity of scientific exchange between this community and ECMI.

Speakers:

P. Mulet. Departament de matemàtica aplicada, Universitat de València (Spain). *Highly accurate weighted extrapolation for finite difference schemes on Cartesian meshes for curved domains.*

M. Dumbser. University of Trento (Italy). *High order ADER schemes for a unified first order hyperbolic formulation of continuum mechanics.*

S. Imperiale. Inria Saclay (France). *Space/time domain decomposition methods for wave propagation simulation.*

C. Parés. Laboratorio de Métodos Numéricos, Universidad de Málaga (Spain). *Well-balanced methods for the Shallow Water equations in spherical coordinates.*

S. Boscarino. University of Catania (Italy). *Semi-implicit method for all mach number flow for the Euler equations of gas dynamics on staggered grid.*

J. Schuetz. Vakgroep wiskunde en statistiek, UHasselt (Belgium). *A novel IMEX splitting for the isentropic Navier-Stokes equations.*

Keywords: hyperbolic systems, conservation laws, shock capturing schemes, numerical methods.

Highly accurate weighted extrapolation for finite difference schemes on Cartesian meshes for curved domains

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The numerical treatment of boundary conditions for partial differential equations is a crucial part for the success of numerical simulations, specially when dealing with curved boundaries. The most common procedure to deal with this task is to use meshes that are adapted to the boundaries, either logically-Cartesian body-fitted meshes or unstructured meshes with or without curved elements (cf. [4, 2]).

For finite difference schemes for hyperbolic equations there have been a number of papers in the literature ([6, 7, 8]) that use extrapolation techniques to handle boundary conditions at curved boundaries. In this contribution we present a new weighted extrapolation technique which improves the techniques presented in [1] for their use for finite difference Weighted Essentially Non Oscillatory schemes [5, 3] applied to hyperbolic problems. This technique is based on the application of a type of Lagrange extrapolation that uses some weights that are computed from smoothness indicators that can implicitly detect regions with discontinuities. We also present a combination of the above technique with a least squares approach in order to stabilize the scheme in some cases where Lagrange extrapolation can turn the scheme mildly unstable. We show that this combined extrapolation technique preserves the order of the underlying scheme and can tackle discontinuities more robustly than the procedure introduced in [1].

Keywords: Finite difference WENO schemes, Cartesian grids, weighted extrapolation.
Acknowledgments. This research was partially supported by Spanish MINECO grants MTM2011-22741 and MTM2014-54388-P.

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High order ADER schemes for a unified first order hyperbolic formulation of continuum mechanics

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This talk is concerned with the numerical solution of the *unified* first order hyperbolic formulation of continuum mechanics recently proposed by Peshkov & Romenski [1], further denoted as *HPR model*. In that framework, the viscous stresses are computed from the so-called *distortion tensor* $\boldsymbol{A}$, which is one of the primary state variables in the proposed first order system. A very important key feature of the HPR model is its ability to describe *at the same time* the behavior of inviscid and viscous compressible Newtonian and non-Newtonian *fluids* with heat conduction, as well as the behavior of elastic and visco-plastic *solids*. Actually, the model treats viscous and inviscid fluids as generalized visco-plastic solids. This is achieved via a stiff source term that accounts for strain relaxation in the evolution equations of $\boldsymbol{A}$. Also heat conduction is included via a first order hyperbolic evolution equation of the thermal impulse, from which the heat flux is computed. The governing PDE system is hyperbolic and fully consistent with the first and the second principle of thermodynamics. It is also fundamentally *different* from first order Maxwell-Cattaneo-type relaxation models based on extended irreversible thermodynamics. The HPR model represents therefore a *novel* and *unified* description of continuum mechanics, which applies at the same time to *fluid mechanics* and *solid mechanics*. In this talk, the direct connection between the HPR model and the classical hyperbolic-parabolic Navier-Stokes-Fourier theory is established for the first time via a formal asymptotic analysis in the stiff relaxation limit.

From a numerical point of view, the governing partial differential equations are very challenging, since they form a large nonlinear hyperbolic PDE system that includes stiff source terms and non-conservative products. We apply the successful family of one-step ADER-WENO finite volume (FV) and ADER discontinuous Galerkin (DG) finite element schemes to the HPR model in the stiff relaxation limit, and compare the numerical results with exact or numerical reference solutions obtained for the Euler and Navier-Stokes equations. Numerical convergence results are also provided. To show the universality of the HPR model, the paper is rounded-off with an application to wave propagation in elastic solids, for which one only needs to switch off the strain relaxation source term in the governing PDE system. We provide various examples showing that for the purpose of *flow visualization*, the distortion tensor $\boldsymbol{A}$ seems to be particularly useful.

Keywords: ADER-WENO finite volume schemes; arbitrary high-order Discontinuous Galerkin schemes; path-conservative methods and stiff source terms; unified first order hyperbolic formulation of nonlinear continuum mechanics; fluid mechanics and solid mechanics; viscous compressible fluids and elastic solids

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Space/time domain decomposition methods for wave propagation simulation

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In this talk we present a space/time domain decomposition strategy for the simulation of linear wave propagation as elastic waves in the context of non-destructive testing (NDT). Numerical simulations of wave propagation play a increasingly important role in NDT tools, e.g. the commercial software CIVA (CEA software platform, see [1]). In this context we present an efficient, flexible and reliable numerical discretization strategy that combines, in one solver, the numerical discretization approaches described below.

Domain decomposition method by mortar element. From a practical standpoint, it allows some flexibility for the construction of configurations (i.e. the description of the geometry and parameters of the problem). From a numerical standpoint, since non-comforming discretizations are allowed, the numerical schemes can be adapted locally to configuration specificities.

Spectral finite elements. The use of conforming high order spectral finite elements methods (see [2]) in each sub-domains is one of the key point for the efficiency of our approach. Since one can achieve mass-lumping without losing accuracy, the use of fully explicit scheme is possible, hence enhancing the efficiency of the numerical schemes in numerous situations. We also present an efficient way to extend the combined use of mortar elements and spectral finite elements as in [3] to the transient case.

Local time-stepping or locally implicit time-schemes. The domain decomposition strategy allows us to use local time stepping (as in [4]) or locally implicit time scheme (as in [5]), hence adapting the time-scheme to the configuration.

Energy preserving time-schemes. When possible and meaningful we aim at ensuring a discrete energy preservation that guaranties the stability in time of our numerical discretizations, thus improving its reliability.

Perfectly matched layer. To efficiently simulate the propagation in unbounded media, among all the techniques available, we use the perfectly matched layer (PML) approach developed in [6] that is specifically adapted to our domain decomposition strategy.

Keywords: Transient wave equation, Domain decomposition, Spectral finite elements, Local time-stepping, mortar elements.

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Well-balanced methods for the Shallow Water equations in spherical coordinates.

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The goal of this work is to obtain first order well-balanced numerical methods and high order extensions for the Shallow Water equations in spherical coordinates:

$$\begin{cases} \dfrac{\partial h}{\partial t} + \dfrac{1}{R\cos(\varphi)}\left[\dfrac{\partial q_\theta}{\partial \theta} + \dfrac{\partial}{\partial \varphi}\left(q_\varphi \cos(\varphi)\right)\right] = 0, \\ \dfrac{\partial q_\theta}{\partial t} + \dfrac{1}{R\cos(\varphi)}\dfrac{\partial}{\partial \theta}\left(\dfrac{q_\theta^2}{h}\right) + \dfrac{1}{R}\dfrac{\partial}{\partial \varphi}\left(\dfrac{q_\theta q_\varphi}{h}\right) + \dfrac{gh}{R\cos(\varphi)}\dfrac{\partial h}{\partial \theta} = \dfrac{gh}{R\cos(\varphi)}\dfrac{\partial H}{\partial \theta}, \\ \dfrac{\partial q_\varphi}{\partial t} + \dfrac{1}{R\cos(\varphi)}\dfrac{\partial}{\partial \theta}\left(\dfrac{q_\theta q_\varphi}{h}\right) + \dfrac{1}{R}\dfrac{\partial}{\partial \varphi}\left(\dfrac{q_\varphi^2}{h}\right) + \dfrac{gh}{R}\dfrac{\partial h}{\partial \varphi} = \dfrac{gh}{R}\dfrac{\partial H}{\partial \varphi}. \end{cases}$$

In this system, R is the Earth radius; g the gravity accelaration; θ and φ the longitude and latitude; h, the thickness of the water layer; H the bottom topography; q_θ and q_φ the components of the discharge in the θ and φ direction respectively. Application of shallow water models to large scale problems (of the order of 1000's of km) requires the use of spherical coordinates: this is the case, for instance, of the simulation of the propagation of a Tsunami wave through the ocean.

Although the PDE system is similar to the Shallow Water equations in cartesian coordinates, the source terms are different. As a consequence, the derivation of numerical methods that preserve water at rest solutions is not as straightforward as in that case. In this work, we first derive a first order path-conservative well-balanced HLL solver on the basis of an adequate choice of variables and a suitable family family of paths. Next, this scheme is extended to a second order well-balanced HLL-WAF method. The extension to well-balanced methods with arbitrary order of accuracy will be also discussed. Some numerical tests will be shown where the properties of the numerical methods are checked.

Keywords: Shallow Water model, well-balanced methods, finite volume methods, approximate Riemann solvers, high order methods.
Acknowledgments. Partially supported by by the Andalusian Government through the project P11-FQM8179.

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Semi-implicit method for all Mach number flow for the Euler equations of gas dynamics on staggered grid

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In this work a numerical method to solve the all-Mach number flow for the Euler equations of gas dynamics on staggered grid is presented. The system is discretized to second order in space on staggered grid, in a fashion similar to the Nessyahu-Tadmor central scheme for 1D model [4] and Jang-Tadmor central scheme for 2D model [5], thus simplifying the flux computation. This approach turns out to be extremely simple, since it requires no equation splitting. We consider the isentropic case and the general case. For simplicity we assume a γ-law gas in both cases. Both approaches are based on IMEX strategy, in which some term is treated explicitly, while other terms are treated implicitly, thus avoiding the classical CFL restriction due to acoustic waves. By rescaling the variables the (possibly small) Mach number ε appears in the equations.

(1) Isentropic Euler Case:

$$\begin{cases} \rho_t + \nabla \cdot (\rho \mathbf{u}) & = 0 \\ (\rho \mathbf{u})_t + \nabla \cdot (\rho u^2 + p/\varepsilon^2) & = 0 \end{cases} \tag{1}$$

completed with the relation $p = k\rho^\gamma$. The core if the implicit term contains a non-linear elliptic equation for the pressure, which has to be treated by a fully implicit technique. Because of the non-linearity, it is necessary to adopt an iterative method to compute the pressure. In our numerical experiments Newton's method worked with few iterations.

(2) General Euler Case:

$$\begin{cases} \rho_t + \nabla \cdot (\rho \mathbf{u}) & = 0 \\ (\rho \mathbf{u})_t + \nabla \cdot (\rho u^2 + p/\varepsilon^2) & = 0 \\ E_t + \nabla \cdot ((E+p)\mathbf{u}) & = 0 \end{cases} \tag{2}$$

The system is closed by the (suitably scaled) equation of state $E = \rho\varepsilon^2 \mathbf{u}^2/2 + p/(\gamma - 1)$. In this case the implicit term is treated in a semi-implicit fashion, thus avoiding the use of Newton's iterations.

In both cases the schemes are implemented to second order accuracy in time. Suitably *well-prepared* initial conditions are considered, which depend on the Mach number ε. In one space dimension we obtain the same profiles found in the literature ([1],[3] for the isentropic case and [1], [2] for the general Euler system) for all Mach numbers. Current work is related on the development of second order accurate schemes for 2D problems and higher order accurate schemes for 1D and 2D problems.

Keywords: Gas Dynamics, All Mach number, Euler Equations, Staggered Grid.

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A novel IMEX splitting for the isentropic Navier-Stokes equations

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In this talk, we consider the isentropic Navier-Stokes equations at low Mach number M. As $M \to 0$, the equation changes its type [5], making it very difficult for numerical methods to work efficiently. This is in particular true for methods of high order consistency. An approach that turns out to be very successful in this context is to split the convective flux into a *stiff* and a *non-stiff* term (see, e.g., [1, 2, 3, 6]), and treat those terms implicitly and explicitly, respectively. (Such an approach is frequently termed IMEX.) We have developed a new splitting based on the $M = 0$ limit solution (*reference solution*, hence termed RS-splitting) and shown its applicability in the context of high-order methods for ODEs [7] and the isentropic Euler equations discretized with first-order Finite Volumes [8, 4]. In this talk, we show how the splitting behaves if spatial discretization is done using the DG method coupled to a high-order IMEX time integration. We present both analytical and numerical results.

Keywords: Navier-Stokes, IMEX, splittings, stability

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MS07: The treatment of singularities and defects in industrial applications

MS07: The treatment of singularities and defects in industrial applications

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Very often industries are interested in removing, and therefore understanding, defects and singularities arising in materials and fluids. In other instances, it is the focusing inherent to singularities and their potential use to manufacture small things what makes them interesting for industrial purposes. This minisymposium gathers researchers who deal with singularities and defects that appear in industrial applications like, for instance, in problems of electro-wetting, superconductivity or dislocations. Such defects are usually undesirable and it becomes crucial to control its origin and evolution. In this sense, many of the topics that are covered in these sessions are at the latest cutting edge. Also, the topic itself is transversal since its industrial motivation ranges from so different fields like fluid dynamics to the allocation of dislocations or superconductivity. Finally, the mathematics involved are usually far from trivial, involving strong nonlinear effects and multiple length and time scales.

Speakers:

Michael Dallaston. Imperial College (UK). *On thin-film rupture with a general disjoining pressure.*

Lia Bronsard. McMaster University (Canada). *On the mathematical study of defects in liquid crystals.*

Hyeonjeong Kim. University of Heidelberg (Germany). *Capillary oscillations at the surface of a fluid in various geometries.*

María Garzón. Universidad de Oviedo (Spain). *Computing through singularities in potential flow with applications to electrohydrodynamic problems.*

David N. Sibley. Department of Mathematical Sciences, Loughborough University, Loughborough (UK). *Uncovering the Nanoscale physics at the moving contact line within a statistical mechanics of fluids framework.*

Keywords: contact line, density functional theory, statistical mechanics, nanofluidics, potential flow, singularities, Level Set method, electrohydrodynamical problems, thin films, self-similarity, rupture, finite-time singularities, nonlinear partial differential equations, calculus of variations, liquid crystals, Landau deGennes, free boundary problem, fluid dynamics, capillary oscillations.

On thin-film rupture with a general disjoining pressure

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A thin film coating a planar horizontal substrate may be unstable to perturbations in the film thickness due to unfavorable intermolecular interactions between the liquid and the substrate. This instability can lead to finite-time rupture of the film. Utilizing the standard lubrication approximation along with the disjoining pressure formalism used to account for the intermolecular interactions [1], the axisymmetric, self-similar nature of rupture at a point has been studied by numerous authors [2, 3, 4] for a particular form of the disjoining pressure with exponent $n = 3$ often used in the literature to account for van der Waals forces. A countably infinite set of similarity solutions exists, of which only one is stable, the one seen in numerical computations of the time-dependent problem [3].

In the present study, we investigate the problem of self-similar rupture for a general disjoining pressure exponent n. We adopt a numerical continuation method implemented in the open source package AUTO-07p [5] to compute many of the discrete self-similar solutions. The same method was recently applied successfully to the plane-symmetric version of this problem with $n = 3$ [6]. Our main finding for general n is that pairs of solution branches merge when n is close to unity; as only the first solution branch is stable to perturbations [3] we expect a critical value n_c below which no stable self-similar solutions exist. This is found to be $n_c \approx 1.485$. This prediction is corroborated by numerical computation of the time-dependent problem; self-similar behavior to point-rupture is observed for $n > n_c$, but when $n < n_c$, the film develops multiple oscillations, and appears to tend toward breakup into multiple rings.

We also numerically evaluate the power-law behavior of characteristic quantities of solutions in the limit of large branch number. The previously computed exponent for $n = 3$ is recovered; however, the analysis performed in [7] indicates that the actual asymptotic result is more subtle, and numerically computed power law estimates must be treated with caution.

Keywords: Thin films, self-similarity, rupture, finite-time singularities
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On the mathematical study of defects in liquid crystals

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The mathematical analysis of liquid crystal models poses many challenging questions, as can be seen by their close relationship to the study of singularities for harmonic maps. In this talk, I will discuss the structure of defects in the context of different models of nematic liquid crystals, and their connection to classical results on harmonic maps into the sphere. To illustrate this, I will present the physically fundamental problem of defects created by a colloid particle immersed in a nematic, and present recent results using the Landau-de Gennes energy. We find that the Landau-de Gennes model allows for a greater variety of types of singularity than the (harmonic map-based) Oseen-Frank energy, including line singularities such as the *Saturn Ring* defect. This is joint work with Stan Alama (McMaster University) and Xavier Lamy (Max Planck Institut, Leipszig)

Keywords: Nonlinear partial differential equations, Calculus of variations, Liquid crystal, Landau-de Gennes functional.
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Capillary oscillations at the surface of a fluid in various geometries

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One of the most classical problems in fluid mechanics concerns the determination of natural frequencies of capillary oscillations by the effects of surface tension. This involves not only multiple possible geometries but also boundary conditions. Many studies have shown the computation of frequencies and solutions of free boundary problems for fluid dynamics. In addition, existence of them has also attracted numerous interests in both fields of mathematics and fluid mechanics.

In this talk, I will discuss the capillary oscillations at the surface of a perfect incompressible fluid constrained in a solid container. Three different geometries are considered for the domain whose boundary consists of the free surface and solid walls of the container. In addition, two different contact line behaviors are considered: the condition that the contact line between free boundary and the solid is pinned and the condition that the contact line can move vertically with a contact angle $\pi/2$.

In all three problems [1, 2, 3], we not only computed frequencies and solutions for the oscillations of the free boundary but also represented them graphically. Results in 2 dimensional cases were extended to other geometries by using a conformal mapping technique. Moreover, we studied the linearized initial value problem [3] and proved well-posedness results in both contact line conditions. As a result, for capillary oscillations when the fluid is in partial contact with a solid as in [3], initial conditions must be prescribed as well as the behavior of the contact line.

Keywords: Partial differential equation, Free boundary problem, Fluid dynamics, Capillary oscillations

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Computing through singularities in potential flow with applications to electrohydrodynamic problems

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Many interesting fluid interface problems, such as wave propagation and breaking, droplet and bubble break-up, electro-jetting, rain drops, etc. can be modeled using the assumption of potential flow. The main challenge, both theoretically and computationally, is due to the presence of singularities in the mathematical models. In all the above mentioned problems, an interface needs to be advanced by a velocity determined by the solution of a surface partial differential equation posed on this moving boundary. A standard approach comes from a Lagrangian-Eulerian formulation of the potential flow equations together with some sort of front tracking method.

This Lagrangian approach is prone to fail when break-up or merging processes appear. Both mathematical and computational difficulties occur when the free boundary changes topology. By using ideas from a level set formulation, the two surface equations of the Lagrangian formulation can be implicitly embedded in PDEs posed in one higher dimension on a fixed domain. The advantage of this approach is that it seamlessly allows topologically breakup or merging of the fluid domain and therefore we provide a computational method when singularities are present in the model.

We present numerical results of a solitary wave breaking, the Rayleigh-Taylor instability of a fluid column, droplets and bubbles breaking-up and the electrical droplet distortion and subsequent jet emission.

Keywords: Potential flow, Singularities, Level Set method, Electrohydrodynamical problems.
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Uncovering the nanoscale physics at the moving contact line within a statistical mechanics of fluids framework

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Understanding the physics in the vicinity of the moving contact line remains one of the unsolved fundamental problems in fluid mechanics. At the heart of the problem is its multiscale nature. Typically, in the viscocapillary regime, three different regions are identified: inner (nanoscale), outer and intermediate region which connects the two. In Ref. [1], we have shown that the inner and the outer region can be connected directly without the need for an intermediate region, therefore dramatically simplifying the asymptotic analysis that has dominated the literature of moving contact lines for several decades.

Here, we unravel the nanoscale physics which alleviates the contact line singularity in the inner region for a single fluid system by employing a dynamic density functional theory (DDFT) approach. The foundation of DDFT is laid on a free-energy formulation based on the statistical mechanics of fluids. The particular DDFT adopted here is a Navier-Stokes-like equation derived in our previous studies [2, 3]. At equilibrium, DFT can be used to obtain the density profile at the contact line as a function of the strength of the wall-fluid interaction [4, 5].

Applying our DDFT to a moving contact line with a no-slip condition at the wall reveals that nanoscale density oscillations in the vicinity of the wall introduce the particle diameter as another crucial length scale to the problem, next to the liquid-vapour interface width. We interrogate the interplay between these two length scales by comparing computations close to the critical and triple points. This is done by analysing the dynamics at different temperatures.

Our DDFT model uncovers a rich dynamic behavior at the nanoscale and, in particular, two interrelated effects are observed: at the length scale of the liquid-vapour interface width, a region of fluid compression is present in the vapour phase, whilst a peak of shear-induced viscous heat production is present in the first particle layers in the vicinity of the wall. We conclude that liquid-vapour phase transition and slip-inducing effects close to the wall are inherently connected for single fluid systems. Results are presented for both advancing and receding contact lines for a wide range of contact angles.

Keywords: contact line, density functional theory, statistical mechanics, nanofluidics.
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MS08: Mathematics in nanotechnology

MS08: Mathematics in nanotechnology

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Nanotechnology is one of the key modern research directions, with billions being invested by governments throughout the world, and in particular by the US, Europe and Japan. Nanotechnology is relevant to a vast range of practical applications, such as in medicine, electronics, biomaterials and energy production. To date the vast majority of research has focussed on the experimental side, with the theory often lagging behind. However, there are a number of mathematical groups now working on topics relevant to the nano industry. In this mini-symposium we intend to bring together a selection of speakers who will discuss a broad range of topics relevant to nanoscience and who will be able to demonstrate the relevance of mathematics to this research field.

Speakers:

Tim Myers and Francesc Font (Centre de Recerca Matemàtica, Spain and University of Limerick, Ireland). *Can you trust mathematics at the nanoscale?*

Helena Ribera (Centre de Recerca Matemàtica, Spain). *Model for nanoparticle melting with a Newton cooling condition and size-dependent latent heat.*

Clemens Heitzinger (TU Wien, Austria). *Stochastic partial differential equations for the modeling of nanowire and nanopore sensors.*

David Gómez-Castro (Complutense University of Madrid, Spain). *Nanocatalysis: homogenization of critical scale two-phase composites with nonlinear reaction.*

Gary O'Keeffe (University of Limerick, Ireland). *Modelling the efficiency of a nanofluid based direct absorption solar collector.*

Keywords: Nanotechnology; Nanofluid; Nanocatalysis; Phase change; Stochastic partial differential equations.

Can you trust mathematics at the nanoscale?

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As in many fields of research mathematics can play a key role but if it is to be truly useful then care must be taken in the development of models that accurately reflect the physics. In this talk we will discuss two areas where mathematical simplifications have led to erronous or unphysical results.

The first part of the talk will deal with the heat transfer of nanofluids. Nanofluids are suspensions of nanoparticles in a base fluid. For a number of years it was suggested that they could be the saviour in the race to find a new, efficient form of cooling fluid (see [1]). However, recent experiments appeared to disprove this. Nevertheless there is still a great deal of theoretical research activity in the field. In particular, practitioners of boundary layer theory, similarity solutions and the Homotopy Analysis Method have published hundreds of papers dealing with different forms of and extensions to a system of equations developed by Buongiorno [2] to describe nanofluid heat transfer. In contrast to the experimental results these authors are almost unanimous in the opinion that nanoparticles have a positive effect on the thermal field and heat transfer characteristics.

We will present a model for nanofluid flow and explain why the mathematical studies contradict the experimental results.

The second part of the talk will deal with the melting of spherical nanoparticles. It is well-known that quantities such as the surface tension, phase change temperature and latent heat vary significantly with size at the nanoscale. However, this is not correctly reflected in the standard governing equations for nanoparticle melting [3]. We will develop a model for the phase change of a nanosphere and highlight the difference to previous models. We will show that differences to the standard model arise due to unphysical assumptions, made for mathematical simplicity, as well as an implicit assumption in deriving the Stefan condition that the enthalpy jump occurs at the bulk melt temperature. Finally, we discuss further modifications involving finite speed heat transfer.

Keywords: Nanofluids; Heat transfer; Phase change; Nanoparticle melting; Stefan problem.
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A model for nanoparticle melting with a Newton cooling condition and size-dependent latent heat

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Nanoparticles have a large ratio of surface to volume atoms which means they have different properties compared to those of the associated bulk material. One example is the well-known decrease in the melt temperature with size as the nanoparticle melts [1]. Surface tension [6] and latent heat [3] also exhibit size dependent effects. For example, Buffat and Borel [1] show a decrease of 500 K for gold nanoparticles slightly bigger than 2 nm in diameter. Lai *et al.* [3] find a reduction of up to 70% in the bulk value of latent heat for tin nanoparticles of 5 nm in diameter.

In the past, mathematical models of nanoparticle melting have neglected the variation in latent heat, whilst including the variation in melt temperature. In this talk we will develop a model that describes the melting of a spherically symmetric nanoparticle which accounts for the reduction in both quantities. Previous approximations [3, 5] of the latent heat variation have used formulae in terms of the inverse of the radius. None of these correctly capture the data for larger nanoparticles. Consequently, we use a novel model, with an exponential dependence which accurately captures the data over a wide range of particle sizes. We also introduce a modified Stefan condition that is appropriate for melting problems at the nanoscale as it takes into account the melting point depression and the surface energy [4]. Finally, we apply a Newton cooling condition at the boundary to drive the melting process. This condition is more realistic than previous theoretical treatments which use a fixed temperature boundary condition. We follow the work of Font *et al.* [2] and include different densities for each phase.

We present both approximate analytical and full numerical solutions to the problem, which show excellent agreement. The inclusion of the modified Stefan condition with size-dependent latent heat results in a substancial decrease in melting times. We show that the dominant factor in this decrease is the size-dependence of the latent heat rather than the different Stefan condition. Nonetheless, the latter factor still has some impact on the final melt time. Comparsion of the fixed temperature boundary condition versus a more realistic Newton cooling condition results in an increase in melting times, which is explained by the initial infinite velocity of the melting front in the case of the former condition.

Keywords: Nanoparticle melting, Mathematical model, Phase change, Numerical simulation.
Acknowledgments. H. Ribera Ponsa has received funding from “la Caixa” Foundation.

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Stochastic partial differential equations for the modeling of nanowire and nanopore sensors

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Introduction. We present recent theoretical and numerical results about stochastic partial differential equations and their application to nanotechnological devices such as nanowire field-effect sensors and nanopore single-molecule sensors [1, 2, 3, 4, 5]. The results primarily concern the numerical stochastic homogenization of elliptic equations, the stochastic Poisson-Boltzmann equation, and the stochastic drift-diffusion-Poisson system.

Methods. For the numerical stochastic homogenization of elliptic equations, we have developed an optimal Monte-Carlo method. It is based on estimating the total approximation error by a sum of three terms. The computational effort of each step in our implementation is measured and gives expressions for the total work. The method is optimal in the sense that the computational work is minimal for a given total error tolerance.

For the Poisson-Boltzmann equation, we have developed a non-intrusive stochastic Galerkin method. Its main advantage is that it is possible to use any existing code for the deterministic Poisson-Boltzmann equation within the Galerkin framework.

For the stochastic stationary drift-diffusion-Poisson system, we show existence and local uniqueness of the solution. We have also devised and implemented an optimal multi-level Monte-Carlo algorithm for this system of equations. Again, the computational effort of each step of solving the system is measured. Then the parameters that minimize the computational effort for a given error tolerance are found. We also perform an optimization of the number of levels and find that there exists an optimal, small number of levels. The levels either are a geometric sequence or are of general fineness.

Results and Conclusions. In the case of the stochastic drift-diffusion-Poisson system, a speed-up of 10^3 to 10^4 of the multi-level approach compared to the straightforward Monte-Carlo method is found for small given error tolerances. To the best of our knowledge, this is the first multi-level Monte-Carlo method for a system of equations.

Keywords: Stochastic partial differential equations, stochastic homogenization of elliptic equations, stochastic drift-diffusion-Poisson system, multi-level Monte-Carlo method, non-intrusive stochastic Galerkin method.
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Nanocatalysis: on the modification of the homogeneized nonlinear chemical kinetics for very small particles

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We study some simplified models arising in nanocatalysis. It is well-known that in many models of Chemical Engineering the theory of homogenization yields a global model given by an effective diffusion and a global interior reaction (the same reaction than holds on the boundary of the pellets) when the size of the particles is assumed to converge to zero (see, e.g., [1] and [2]). It is assumed, usually, that the size of the particles is of the same order as their repetition. In this talk we aim to give a rigorous presentation of further results when the size of the particles is very small. As in other domains of the nanotechnology new and unexpected behaviors arise.

Let us introduce the following model for a *fixed bed reactor*:

$$\Omega_\varepsilon = \Omega \setminus \bigcup_{i\in\Upsilon(\varepsilon)} (\varepsilon i + \varepsilon^\alpha G_0), \qquad \Upsilon(\varepsilon) = \{i \in \mathbb{Z}^n \mid d(\varepsilon i + \varepsilon^\alpha G_0, \partial\Omega) > 2\varepsilon\} \tag{1}$$

where G_0 is the shape of a reactive particle, a bounded open set of $\mathbb{R}^n$ and $\alpha \geq 1$ is the relation between the size of the particles and their repetition. Let us consider a nonlinear diffusion operator and nonlinear reaction model where reaction takes place in the boundary of the particles, S_ε:

$$-\Delta_p u_\varepsilon = f,\ \Omega_\varepsilon, \qquad u_\varepsilon = 0,\ \partial\Omega, \qquad \partial_{\nu_p} u_\varepsilon + \varepsilon^{-\gamma}\sigma(u_\varepsilon) = 0,\ S_\varepsilon = \bigcup_{i\in\Upsilon(\varepsilon)} \partial(\varepsilon i + \varepsilon^\alpha G_0), \tag{2}$$

where σ is (for simplicity) a continuous increasing function. Here, as we will show, the good choice is $\gamma = \alpha(n-1) - n$. The aim of this talk is to present some new results (some of them obtained in collaboration with A.V. Podol'skii and T.A. Shaposhnikova) classifying three well differenced dynamics in the limit, that is the limit u of the sequence u_ε as $\varepsilon \to 0$:

- If $\alpha = 1$, $p = 2$ (see [2]) then a effective diffusion and a global interior reaction appears $-\mathrm{div}(A_0\nabla u) + \lambda\sigma(u) = f$.
- If $1 < \alpha < \frac{n}{n-2}, 1 < p < n$ then no effective diffusion appears and $-\Delta_p u + \mu\sigma(u) = f$.
- If $\alpha = \frac{n}{n-2}, 1 < p < n$ then the nature of the non linearity changes and $-\Delta_p u + \rho H(u) = f$. Here H is an increasing function associated to σ through a suitable functional equation.

The third case can be seen as a mathematical formulation of some *unusual catalytic behavior* found in some experiments in nanocatalysis (see, e.g. [3]). As a matter of fact, to find some mathematical justification of such unusual behaviour was an important part of the motivation of our study.

Keywords: semilinear elliptic equations, homogenization, nanotechnology, chemical engineering

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Modelling the efficiency of a nanofluid based direct absorption solar collector.

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The Sun provides Earth with more energy every hour than all of human civilisation uses in one year. No other energy supply is as plentiful as the 120,000 terawatts the Sun provides ceaselessly and unbidden. The solar energy industry has experienced phenomenal growth in recent years due to both technological improvements resulting in cost reductions and government policies supportive of renewable energy development and utilisation [1]. Unlike traditional direct absorption solar collectors (DASCs), nanofluid-based direct absorption solar collectors (NDASCs) use a colloidal solution of nanoparticles and a base fluid to absorb incident sunlight. This method increases efficiency over flat plate solar collectors and DASCs [2,3]. The actual theoretical increase in efficiency is unclear and depends on the mathematical assumptions made during the modelling process. In this talk we present an approximate analytical solution to the steady state, two-dimensional model for the efficiency of a NDASC.

The model consists of a system of partial differential equations describing the conservation of mass, momentum and energy, in the particular case of nanofluids moving within a solar energy installation. By applying the method of separation of variables to the equations describing the conservation of mass we find a depth dependent velocity profile in the nanofluid. A heat source term is obtained via the radial flux integral, which is highly non-linear with respect to wavelength due to the spectral-dependent fluid and nanoparticle indices of refraction and absorption. To make analytical progress we introduce an approximate power-law function for the radial flux. This approximation of the integral can also be found in similar research [4]. Applying the method of separation of variables, the resulting solution is used to investigate the efficiency of the collector subject to variation in model parameters. We assume the velocity of the nanofluid in the solar collector is depth dependent while other authors assume the velocity is constant [4]. In spite of this added level of complexity, we are still able to solve the problem analytically. We also discuss the extension to a three dimensional model in a cylindrical pipe. This approach adds considerable complexity, and the problem must be solved using a finite difference scheme.

Keywords: Nanofluid; direct absorption solar collector; solar energy; efficiency; heat; diffusion equation.
Acknowledgments. G. O'Keeffe was supported by an Irish Research Council grant GOIPG/2014/887.

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MS09: Aeroacoustics

MS09: Aeroacoustics

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Aeroacoustics can be seen as a branch of fluid mechanics that deals with the propagation of acoustic waves in moving fluids (flows). There are obviously many industrial applications of aeroacoustics to begin with aeronautics and car industry (controlling the noise emitted by airplanes and cars is definitely a major issue) but also the control of noise in domestic ducts like air-conditioning for instance.

As a consequence, understanding in depth sound propagation in flows and being able to simulate numerically the corresponding physical phenomena are two major issues that represent scientific challenges for applied mathematicians. Even one could think that computational aeroacoustics is only a part of computational fluid dynamics, as a matter of fact, the modelization of acoustics in flows is a discipline of its own right. Indeed, taking into account the small proportion of mechanical energy involved in the production of sound, one traditionally uses mathematical models issued from various versions of the linearization of full nonlinear models, such as Euler of Navier-Stokes equations, around a reference flow that is most often considered as stationary (time independent) at the time scales of interest.

Dealing with such models from both mathematical and computational points of view raises new interesting and non trivial questions.

The first one is the choice of a mathematical model and the design of a corresponding numerical method, the two aspects being intimately linked. Indeed, many "equivalent" models are available (Linearized Euler Equations, Galbrun's equations, Golstein's equations, Möhring's equations, ...) and lead to various simplifications according to particular properties of the reference flow (laminar flow, potential (or irrotational) flow, ...). These models mainly differ by the choice of the unknowns that are used but also in their mathematical form that is more or less well adapted to a given mathematical (for the analysis) or numerical (for simulation) approach. These choices will also be guided by the fact that one is interested in a transient problem (in this case, one treats an evolution problem in which time is a variable) or in a time harmonic problem (one looks for a solution that oscillates in time at a given frequency). In the recent past years, various numerical methods have been developed around the use of continuous or discontinuous Galerkin methods for space discretization and, when needed, finite differences in time. Such methods are still the object of various improvements and their analysis still raise open questions.

A second very important question is the treatment of boundary conditions. This question can be divided into two parts. The first one concerns physical boundaries that is related to the interaction of acoustic waves with walls. The second one is related to artificial boundaries introduced for bounding the computational domain. In the first case, various effective boundary conditions (whose expression is, by the way, influenced by the choice of the "interior" model) have been recently proposed to take into account thin boundary layers as well as absorbing walls. Their use raises delicate questions related to the well-posedness and stability analysis of the corresponding boundary value problems. In the second case, which also raises difficult stability questions, several existing methods are competing, including Perfectly Matched Layers or time domain integral equations (retarded potentials).

The aim of this mini-symposium is to propose to give an overview of the state of the art around these questions and to emphasize the most recent developments in the domain.

Speakers:

J. F. Mercier. POEMS, CNRS-INRIA-ENSTA (France) *A brief review on some open questions in aeroacoustics modeling.*

C. Legendre. Free Field Technologies (Belgium) *Effects of non-uniform mean flows on sound propagation using scalar operators.*

A. Semin. Technische Universität Berlin (Germany) *Asymptotic modelling of the wave-propagation over microperforated absorbers.*

A. Bensalah. POEMS, CNRS-INRIA-ENSTA *Introduction to the Goldstein Model in aeroacoustics.*

J. Chabassier. INRIA Bordeaux (France) *Solution of time-harmonic Galbrun's equation in the context of helioseismology.*

J. Rodríguez. Universidade de Santiago de Compostela (Spain) *Boundary integral equations and discontinuous Galerkin methods for transient aeroacoustics.*

A brief review on some open questions in aeroacoustics modeling

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Our aim is to give an introduction to Aeroacoustics, to describe the state of the art and to emphasize the most recent developments. Two major issues for applied mathematicians in Aeroacoustics are to understand the sound propagation in flows and to be able to simulate numerically the corresponding physical phenomena. The usual mathematical models are issued from various versions of the linearization of full nonlinear models, such as Euler or Navier-Stokes equations, around a reference stationary flow. Dealing with such models from both mathematical and computational points of view raises interesting and non trivial questions.

A first one is the choice of a mathematical model and the design of a corresponding numerical method. Indeed, many "equivalent" models are available (Linearized Euler Equations, Galbrun's equation, Golstein's equations, Möhring's equations [1], ...). These models mainly differ by the choice of the unknowns that are used but also in their mathematical form that is more or less well adapted to a given mathematical approach for the analysis or a numerical approach for the simulation. These choices are also guided by the fact that one is interested in a transient problem [2] or in a time harmonic problem.

A second important question is the treatment of boundary conditions and this question can be divided into two parts. The first one concerns physical boundaries and is related to the interaction of acoustic waves with walls. Various effective boundary conditions have been recently proposed to take into account absorbing walls in presence of a grazing flow,[3, 4] as well as thin boundary layers [5]. Their use raises delicate questions related to the well-posedness and stability analysis of the corresponding boundary value problems. The second question is related to artificial boundaries introduced for bounding the computational domain and also raises difficult stability questions. Several existing methods are competing, including Perfectly Matched Layers or time domain integral equations (retarded potentials) [6].

Keywords: models in aeroacoustics, impedance boundary condition, transparent boundary conditions

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Effects of non-uniform mean flows on sound propagation using scalar operators

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The **L**inearized **N**avier-**S**tokes **E**quations (**LNSE**) are the reference operator for linear acoustic propagation predictions. This is because the number of effects that are taken into account, namely: (i) classic acoustic propagation; (ii) mean flow effects (convection, dilatation and rotational effects); (ii) temperature effects via a space-variable speed of sound and density; and (iv) visco-thermal dissipative effects. Since the **LNSE** are represented by five linear partial differential equations coupled in time and space, the numerical methods for solving such equations in industrial applications represent a significant cost, that in most cases is prohibitive.

The present symposium deals with mathematical and physical approximations that make the **LNSE** (vector operator) degenerate to scalar wave operators of second order in space and any order in time. The main advantages of having a scalar wave operators are: (i) better physical interpretation of each term of the wave operator; (ii) less sensitivity to acoustic instabilities (Kelvin-Helmholtz); (iii) well adapted to classic finite element method discretization and non-reflecting boundary conditions such as **PMLs** (**P**erfect **M**atched **L**ayers) and infinite elements [1]; and (iv) combination of the operators in different regions of space (numerical modularity, multi-physics) to better asses the wave phenomenon prediction.

The scalar operators to be presented in the symposium are listed follows as: (i) Helmholtz's operator: acoustic propagation in a fluid at rest, based on pressure terms; (ii) Pierce's Operator: wave operator in an inhomogeneous fluid at rest [2], based on pressure terms; (iii) Möhring's operator: wave operator in an inhomogeneous fluid with convection (potential flow), based on total enthalpy terms [3]; (iv) **F**amily of **W**eakly **C**oupled **A**coustic-**V**ortical **W**ave **E**quations (**FWCAWE**): wave operators in an inhomogeneous fluid with convection (potential and rotational flow), based on total enthalpy terms [4, 5]; (v) e**X**tended **L**ow **R**educed **F**requency model (**XLRF**): wave operator in a dissipative (viscous) media with constant convection within waveguides, based on pressure terms [6]; and (vi) Distance-based model for visco-thermal wave propagation: wave operator in a dissipative (viscous) media at rest for arbitrary (3D) geometries, based on pressure terms [7]. The operators presented above can be mathematically condensed in a single **G**eneric **S**calar **W**ave **O**perator (**GSWO**) with coefficients depending on the phenomena's predictions required.

Keywords: Wave operators, acoustics, inhomogeneous media.

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Asymptotic modelling of the wave-propagation over microperforated absorbers

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We will consider the acoustic wave propagation in a channel separated from a chamber by a thin periodic layer. This model stands for microperforated absorbers, which are used to supress reflections from walls. Due to the smallness of the periodicity a direct numerical simulation, e.g. with the finite element method (FEM), is only possible for very large costs. Based on homogenization techniques we find impedance transmission conditions [2], which integrated into numerical methods like the FEM or the boundary element method leads to much lower computational costs. For microperforated absorbers of finite length their endings have a significant impact to the macroscopic absorption and this effect is a-priori not considered with the transmission conditions. We aim to describe the interaction of the thin periodic layer with the singularities from its endings asymptotically when the periodicity and layer thickness δ tend to zero [5]. For this, the Kondratiev theory for corner singularities (which is based on the Mellin transform) has to be extended to infinite cones with periodic layers [4] by techniques similarly to those developed in [3].

Keywords: Microperforated absorbers, transmission conditions, corner singularities.
Acknowledgments. Partially supported by the Einstein foundation Berlin (project IFP-2011-98).

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Introduction to the Goldstein model in aeroacoustics

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Introduction to the Goldstein model. We are interested in modeling the acoustic radiation in a complex air flow, considered as a perfect isentropic gaz, in the time harmonic domain. In aeroacoustics, the 0-order hydrodynamic problem, which corresponds to the stationary Euler equations, provides the pressure p_0 and the velocity $\boldsymbol{v_0}$ of the so-called carrier flow. Others quantities as the sound speed c_0 are then deduced. Aeroacoustic models correspond to the first order linearization of Euler equations around the carrier flow $(\boldsymbol{v_0}, p_0)$ and have for unknowns the first order perturbation quantities, namely the acoustic pressure p and the acoustic velocity $\boldsymbol{v}$. For a potential carrier flow, one can show [1] that the acoustic velocity also derives from a potential φ (s.t. $\boldsymbol{v} = \boldsymbol{\nabla}\varphi$) which satisfies the convected Helmholtz equation. We present a generalization where $\boldsymbol{v_0}$ is no longer supposed to be potential. Nevertheless, one shows that [2] there exists a couple of unknowns $(\varphi, \boldsymbol{\xi})$ generalizing in a certain meaning the potential model. The scalar unknown φ satisfies a convected Helmholtz like equation whereas the vectorial unknown $\boldsymbol{\xi}$ satisfies a transport like equation, both coupled, namely the Goldstein model

$$\rho_0 D\Big(\frac{1}{c_0^2} D\varphi\Big) - \boldsymbol{\nabla}\cdot(\rho_0 \boldsymbol{\nabla}\varphi) = f + \boldsymbol{\nabla}\cdot(\rho_0 \boldsymbol{\xi}) \quad \text{and} \quad D\boldsymbol{\xi} + \boldsymbol{\xi}\cdot\boldsymbol{\nabla}\boldsymbol{v_0} = \boldsymbol{\nabla}\varphi \times \boldsymbol{\omega_0}, \tag{1}$$

where $D := -i\omega + \boldsymbol{v_0}\cdot\boldsymbol{\nabla}$ denotes the time harmonic convective derivative and $\boldsymbol{\omega_0} = \mathbf{curl}(\boldsymbol{v_0})$ is the vorticity of $\boldsymbol{v_0}$. From $(\varphi, \boldsymbol{\xi})$, we retrieve the classical acoustic pressure $p = -\rho_0 D\varphi$ and the acoustic velocity $\boldsymbol{v} = \boldsymbol{\nabla}\varphi + \boldsymbol{\xi}$ [2]. In aeronautic applications as jet flows for instance, areas where the vorticity is non-negligible are restricted. Compute $\boldsymbol{\xi}$ only on these restricted areas allows significant computationnal costs saving.

Well-posedness. In general, the well-posedness of the Goldstein model is a delicate issue. We assume that $\boldsymbol{v_0}$ is Ω-filling i.e. almost every point of Ω is reached by a streamline of $\boldsymbol{v_0}$ started from the inflow boundary in a uniformly bounded time. Within this framework, we are able to establish a coercive weak formulation of the Goldstein model if the carrier flow is subsonic as in the potential case, but also if its gradient is sufficiently small. The situation is much more complicated when the flow is not Ω-filling, especially when closed streamlines of $\boldsymbol{v_0}$ exist. In particular, we evidence the existence of resonant pulsations of the transport equation along some closed lines in some toy cases.

Numerical approach. We present a numerical method to solve the Goldstein model in the Ω-filling case, combining a classical continuous Galerkin method for φ and a Streamline Upwind Petrov Galerkin method [3] for $\boldsymbol{\xi}$.

Keywords: aeroacoustics, Goldstein model, well-posedness, resonance frequencies, Finite Elements Method.

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Solution of time-harmonic Galbrun's equation in the context of helioseismology

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When gravitational and magnetic forces are neglected, the propagation of acoustic waves inside the Sun can be modelled with Galbrun's equation (in time-harmonic domain):

$$\rho_0 \left(-i\omega + \sigma + M\cdot\nabla\right)^2 u - \nabla\left(\rho_0\, c_0^2 \,\mathrm{div}\, u\right) + (\mathrm{div}\, u)\,\nabla p_0 - (\nabla u)^T \nabla p_0 \;=\; f \tag{1}$$

where ρ_0, c_0, p_0 are the background density, sound speed and pressure, σ is a damping coefficient. For a quiet sun, the flow $M = (m_x, m_y)$ is null, but is non-null in the general case. In this talk, we will explore different formulations in order to solve Galbrun's equations in 2-D and for an axisymmetric geometry. Equation (1) will be solved directly with SIPG (Symmetric Interior Penalty Galerkin) method. An equivalent first-order formulation can be easily obtained

$$\begin{cases} \rho_0\left(-i\omega + \sigma + M\cdot\nabla\right) u - \rho_0 v = 0, \qquad p - \mathrm{div}\, u = 0 \\ \rho_0\left(-i\omega + \sigma + M\cdot\nabla\right) v - \nabla(\rho_0\, c_0^2\, p) + p\nabla p_0 - (\nabla u)^T\nabla p_0 = f \end{cases}$$

This formulation will be solved with LDG (Local Discontinuous Galerkin) method. The equation for p of this formulation is similar to a constraint. In order to obtain a formulation close to an hyperbolic system, we have introduced the following first-order formulation

$$\begin{cases} \rho_0\left(-i\omega + \sigma + M\cdot\nabla\right) u - \nabla p - \rho_0\, q = 0, \qquad \rho_0\left(-i\omega + \sigma + M\cdot\nabla\right) p - \rho_0^2\, c_0^2\, \mathrm{div}\, u = 0 \\ \rho_0\left(-i\omega + \sigma + M\cdot\nabla\right) q - (\nabla\sigma)\, p - (\nabla M)^T\nabla p - \dfrac{M\cdot\nabla\rho_0}{\rho_0}\nabla p + (\mathrm{div}\, u)\nabla p_0 - (\nabla u)^T\nabla p_0 = f \end{cases}$$

This equivalent formulation will be solved with LDG as well. Finally, a H^1 formulation (coupled with discontinuous Galerkin) [1] has been considered. All these formulations are equivalent and should provide the same solution. Linearized Euler Equations are also considered, they give the same solution as Galbrun's equations for an uniform flow and when $f \;=\; (-i\omega + \sigma + M\cdot\nabla)g$.

$$\begin{cases} (-i\omega + \sigma + M\cdot\nabla)p + \mathrm{div}(c_0^2\, u) + (\gamma-1)(\mathrm{div} M)\, p - \dfrac{(\gamma-1)}{\rho_0} u\cdot\nabla p_0 = 0 \\ (-i\omega + \sigma + M\cdot\nabla)\rho + \rho\,\mathrm{div}\, M + \mathrm{div}\, u = 0 \\ (-i\omega + \sigma + M\cdot\nabla)u + \nabla p + \nabla M(u + \rho\, M) = \dfrac{g}{\rho_0} \end{cases}$$

When the flow is uniform (or null), the different formulations converge correctly in a similar fashion. Tests have been conducted on a square domain with periodic coefficients. When the flow is small, the different formulations seem to converge correctly, but it is no longer the case for larger values of the flow. This default of convergence is not observed for Linearized Euler Equations. Simplified Galbrun's equations are derived by neglecting certain terms, such that they are equivalent to Galbrun's equation when M is null, and converge nicely. They are solved for realistic coefficients of the sun with a rotating flow. While original Galbrun's equations exhibits curious oscillations that are not converged, this new formulation gives a satisfying solution.

Keywords: Galbrun's equation, Discontinuous Galerkin, Helioseismology.

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Boundary integral equations and discontinuous Galerkin methods for transient aeroacoustics

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In this work we are interested in the numerical simulation of acoustic waves in the presence of a flow on unbounded domains. To model this phenomena we consider the following set of equations

$$\left|\begin{array}{rcrcl} \dfrac{\partial p}{\partial t} & + & \boldsymbol{M}\cdot\nabla p & + & \operatorname{div}\boldsymbol{v} = f, \\ \dfrac{\partial \boldsymbol{v}}{\partial t} & + & \boldsymbol{M}\cdot\nabla \boldsymbol{v} & + & \nabla p = \boldsymbol{g}, \end{array}\right. \tag{1}$$

where $\boldsymbol{M}$ is the flow that is assumed to be uniform in the complementary region of a bounded domain Ω_i. This raises the question of bounding the computational domain and, at the same time, accounting for the heterogeneities of the coefficients. In this work we propose to use transient boundary integral equations [2] to handle the unbounded nature of the computational domain and a discontinuous Galerkin method [3] in space combined with finite differences in time to account for the presence of a (eventually) non-uniform flow. Both techniques are coupled using an extension of the coupling algorithm introduced in [1] for the scalar wave equation. This extension allows to discretize not only the model in (1) but any symmetric hyperbolic Friedrichs system and permits the use of a large variety of numerical fluxes in the interior domain.

Keywords: Retarded potentials, discontinuous Galerkin methods, coupling techniques, stability, Friedrichs systems, aeroacoustics.

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MS10: Simulation and optimization of water and gas networks

MS10: Simulation and Optimization of water and gas networks

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In this minisymposium the fluid flow of water and gas through large networks will be treated. These networks can consist of rivers or channels, gas and water supply or sewer systems. The flow in one single network element is usually modelled by hyperbolic conservation laws or some simplifications. All single flow reaches must be coupled by appropriate coupling and boundary conditions. This approach leads to PDAEs (partial differential algebraic equations) and requires very robust and efficient numerical methods for their solution. Moreover, the optimization of the network operation with respect to the security of supply or energy consumption is of importance. Suitable optimization methods for these requirements are an active field of research.

Speakers:

T. Clees, K. Cassirer, B. Klaassen, I. Nikitin, L. Nikitina. Fraunhofer-Institut für Algorithmen und Wissenschaftliches Rechnen SCAI (Germany). *A new NLP analyzer and solver for gas networks with compressor stations.*

A. Bermúdez, X. López and M.E Vázquez-Cendón. Universidade de Santiago de Compostela (Spain). *Finite volume schemes for solving transient models of gas transportation networks.*

Y. Lu, J. Mohring, N. Marheineke. Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM (Germany). *Matrix interpolation for parametric MOR of gas pipeline networks.*

G. Steinebach. Hochschule Bonn-Rhein-Sieg (Germany). *TWaveSim - a simulator for water works and supply networks.*

L. Wagner. Technische Universität Darmstadt (Germany). *Second order implicit schemes for solving balance laws with applications to water supply networks.*

B. Liljegren-Sailer, N. Marheineke. Friedrich-Alexander-Universität Erlangen-Nürnberg (Germany). *Structure preserving MOR for gas networks with active elements.*

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A new NLP analyzer and solver for gas networks with compressor stations

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Natural gas pipeline systems are an essential part of our energy supply. Systems can have several thousands of kilometers of pipes and several thousands of network elements such as pipes, valves, regulators, compressors etc. For simulation, they can be modeled based on isothermal Euler equations. The isothermal Euler equations form a coupled system of PDEs consisting of mass and momentum balance laws together with a constitutive relation. De facto, nonlinear ODE or DAE systems are usually solved in practice. Our MYNTS software computes several fields in space (steady-state mode) or space-time (time-dependent mode), namely for pressure, mass flow (volume flow, power), temperature, and 21 main components of natural gas.

In this talk, we address several issues when solving practical applications, including modeling aspects, graph analysis, hierarchical coarsening, acceleration and robust (Pareto) optimization. We outline solution methods and discuss some novel methods, realized in MYNTS, in more detail.

In particular, we present a new approach for efficiently solving nonlinear problems arising here by means of an NLP solver based on an interior-point method with an adapted line search algorithm. This method has originally been developed for piecewise linear systems. Our tests show that it also works for slightly non-linear piecewise smooth ones as well.

The main idea stems from methods for solving nonlinear resistor networks in electrotechnics [1, 2]. This covers, for instance, voltage-increasing elements such as batteries with internal resistance. Some elements in the networks considered are modeled by non-smooth equations. Among them are diodes. They are approximated by piecewise linear functions. In case of gas transport systems, exemplary analogues to the above-mentioned elements are compressors (they increase pressure), as well as regulators, flaptraps, pressure-drop-type resistors etc.

It can be shown that, under relevant conditions, there is a single solution of the system which can be found with a special line search algorithm. In our case, the control equations for regulators and compressors possess a piecewise linear form in max-min/abs-normal representation [3]. They define a polyhedral surface the faces of which correspond to elementary states. Voronoi subdivision defines the regions used in the line search procedure developed.

Keywords: gas transport, NLP solvers, graph analysis, coarsening, Pareto optimization.

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Finite volume schemes for solving transient models of gas transportation networks

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Managing gas transport networks is a complex problem because of the great number of possibilities to routing the gas through the pipes. Thus, mathematical modelling is an important subject in planning and operating gas transportation networks (see reference books, [6] [7]). Most papers and computer programs on the subject deal with the case of steady state. Based on steady state models, network optimization problems have been considered that, in particular, aim at saving operation costs related to the self consumption of gas in compression stations, needed to compensate the pressure loss due to pipe wall friction (see [1] [8]). However, less papers have been devoted to transient models (see, for instance, [4] [5]); besides they only consider one single pipe, not a network, and asssume isothermal or isentropic flow of perfect gases.

The present work deals with transient mathematical modelling of gas transport networks including compressor stations and control valves. The model consists of a system of nonlinear hyperbolic partial differential equations coupled at the nodes of the network whose topology is modelled by a direct graph. The edges of the graph represent pipes where the gas flow is modelled by the non-isothermal non-adiabatic Euler compressible equations for real gases, with source terms arising from heat transfer with the outside of the network, wall viscous friction, and gravity force; the latter involves the slope of the pipe.

Regarding numerical solution, for each pipe a finite volume scheme is introduced (see also [2]). In order to make an upwind discretization of the flux, the Q-scheme of van Leer is used. Moreover, to get a well-balanced scheme the source terms are discretized by making some upwinding similar to the one in the flux term proposed in ([3]). Moreover, the numerical coupling at junctions is also addressed.

Keywords: Gas flow in transportation networks, nonlinear hyperbolic systems with sources, finite volume method, well-balanced schemes.

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Matrix interpolation for parametric MOR of gas pipeline-networks

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A method is presented for interpolating Balanced Truncation-based parametric reduced order models (BT-pROM) in oder to approach BT-pROMs at a new parameter set by counterparts at a given parameter set. This method is extended from the general framework for model order reduction (MOR) for high-order parameter-dependent linear time invariant systems (LTIS) in descriptor form proposed in [1] and treats not only permutations and rotations but also distortions of reduced order basis (ROB) vectors. Furthermore, its applicability is shown on BT-pROMs for gas transport in a pipeline-network.

Keywords: matrix interpolation, parametric model order reduction, balanced truncation, gas pipeline-network.

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TWaveSim - A Simulator for water works and supply networks

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Reliable supply of drinking water for the population is of great importance. In this context, besides the required water quality energy efficiency becomes an increasing issue for water supply companies. In order to optimize corresponding interplay between energy consumption for pump operation and satisfaction of water demands, a dynamical mathematical simulation of hydraulics and energy is required.

For realizing such computations, simulator TWaveSim was developed. It is based on special modelling approaches for processes of water extraction and treatment in water works and subsequent dissemination into large networks. TWaveSim allows for different modes such as simulation and forecast. In simulation mode the adaption to measured tank levels is possible. Single model elements like pumps, valves, pipes, tanks etc. are described by linear or nonlinear equations as well as ordinary or partial differential equations. The simulator collects all occurring modelling equations and coupling conditions into one large DAE system by applying an appropriate network approach using the method of lines and suitable semidiscretization of given hyperbolic PDEs [1, 2].

In this talk, simulator TWaveSim is introduced in detail. Implemented equations for pipes, control valves and speed controled pumps are presented and the special structure of the resulting DAE system is discussed. This structure must be exploited by the proposed linearly-implicit Rosenbrock-Wanner (ROW) methods [3, 4] for time-integration of the given DAE system. Finally, some simulation and forecast results will be presented and discussed as well.

Results show dynamical flow behaviour within single reaches and thus motivate applying generalized ROW-type methods [5] in order to further increase efficency of time-integration. Corresponding considerations are subject of Tim Jax's talk "Generalized ROW-Type Methods for Simulating Water Supply Networks".

Keywords: Water supply network simulation, network approach, method of lines, DAEs
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Second order implicit schemes for solving balance laws with applications to water supply networks

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The today's demands for simulation and optimization tools for water supply networks are permanently increasing. Practical computations of large water supply networks show that rather small time steps are needed to get sufficiently good approximation results – a typical disadvantage of low order methods. Having this in mind we use higher order time discretizations to overcome this problem. Such discretizations can be achieved using so-called SSP (strong stability preserving) Runge-Kutta methods [2] which are especially designed for hyperbolic problems. Therefore we use a second-order two-stage SSP-SDIRK (singly-diagonally implicit Runge-Kutta) method [3]. Being an implicit time integration, the SDIRK method appropriately handles dissipative source terms which become important when modeling water flow in pipes [1]. Further structural advantages make the schemes superior to general fully implicit Runge-Kutta methods in terms of computation time.
Our intention is to compare different space discretizations and combine them with the SDIRK method to get fast and stable numerical schemes for solving hyperbolic problems. For the space discretizations we aim at approximating weak entropy solutions which are based on variational formulations. In this talk we will present numerical and first theoretical results considering hyperbolic balance laws.

Keywords: hyperbolic balance laws, strong stability preserving Runge-Kutta methods, water supply networks

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Structure preserving MOR for gas networks with active elements

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We consider gas networks and aim for an efficient simulation with the help of Model Order Reduction (MOR) tools. Gas networks are modeled as coupled systems of nonlinear partial differential and algebraic equations. They mainly consist of pipes, but other components like compressor stations and valves have to be considered as well.
In our approach we identify connected pipe-only subnetworks and create low-order surrogate models for them to speed up the overall simulation. The dynamics of the pipes is modeled by a semilinear simplification of the Euler-equations with friction. Together with boundary and coupling conditions this leads to a partial differential algebraic equation of hyperbolic type. The system is first appropriately space-discretized, and then examined with index- and decoupling-concepts for differential algebraic equations. For the arising input-output system we construct explicit representations of strictly proper part, only depending on the topology. We seek for surrogate models of this strictly proper part. In this talk the capability of structure preserving MOR will be shown for systems with a simplified linear pipe flow model. A comparison to a direct simulation is done for networks with active elements.

Generalized ROW-type methods for simulating water supply networks

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In order to supply drinking water efficiently, aspects such as saving energy and resources become more and more relevant besides the task of ensuring water quality. In this context, simulating water supply networks is of increasing importance as it helps water suppliers to estimate and improve effectiveness of their facilities with respect to economy and ecology. However, modeling and computing meaningful water supply systems is demanding. It requires to take into account processes for procurement and preparation of water within water works as well as its subsequent distribution in large networks. As a consequence, resulting mathematical systems prove to be correspondingly complicated and thus require research in efficient and robust numerical methods.

In more detail, pressurized water transport in closed pipes must be considered for these simulations that is generally modeled by hyperbolic PDEs such as the water-hammer equations. In addition, linear and non-linear algebraic constraints as well as supplementing ODEs are included to describe boundary and coupling conditions of single reaches or components such as pumps and valves given within a network, thus leading to an extensive PDAE system. An established approach to solve such problems is the method of lines that, based on spatial semi-discretization, finally yields a large DAE system.

Linearly implicit Rosenbrock-Wanner (ROW) methods proved to be robust and efficient solving such DAE systems [4]. But as flow behavior within networks for water supply is observed to be quite dynamical their computational effort is assumed to be significantly reduced by applying partial explicit integration of underlying Runge-Kutta (RK) schemes. Besides, further effort might be reduced by decreasing the number of costly Jacobian computations that are usually required with every time-step.

Combining ROW and RK schemes as well as avoiding a ROW method's Jacobian computation with every time-step is well-defined for ODE problems by so-called W methods [3]. Corresponding extensions to the DAE case are covered by generalized ROW-type methods [2]. Generalized ROW-type methods proved to be quite promising regarding first applications to simplified test problems of dynamical free-surface flow in single reaches [1]. In this contribution, we analyze advantages of these methods compared to standard ROW schemes when simulating pressurized flow in water supply networks. For this purpose, we apply schemes that consider both partial explicit integration as well as reduced Jacobian calculations in order to decrease computational effort effectively.

Keywords: Rosenbrock-Wanner methods, W methods, DAEs, implicit-explicit strategies
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MS11: Mathematical modeling and simulation for nano-electronic coupled problems (nanoCOPS)

MS11: Mathematical modeling and simulation for nanoelectronic coupled problems (nanoCOPS)

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In this minisymposium recent advances in mathematical modeling, uncertainty quantification (UQ) and model order reduction (MOR) for electronic devices are presented. They are the research results from the cooperation between the academic and industrial partners in the framework of nanoCOPS ('Nanoelectronic Coupled Problems Solutions'). It is a collaborative research project within the research program 'Information and communication technologies' (of the Seventh Framework Programme for Research and Technological Development (FP7) funded by the European Union.

The project addresses the development of efficient simulation/design tools for Power-MOS devices, with applications in energy harvesting, that involve couplings between electromagnetics, heat, and stress, and radio-frequency circuitries in wireless communication, which involves electro-thermal coupling, electromagnetic-circuit-heat coupling and multirate behaviour, together with analogue-digital signals. Efficient mathematical modeling, UQ and MOR approaches act as important roles in the design processes, and will be the focus of this minisymposium.

Speakers:

Roland Pulch, Piotr Putek, Herbert de Gersem. Universität Greifswald (Germany), Bergische Universität Wuppertal (Germany) and Technische Universität Darmstadt (Germany). *Identification of probabilistic input data for modeling uncertainties.*

Nicodemus Banagaaya, Peter Benner and Lihong Feng. Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg (Germany). *PMOR for Linear Systems with Many Inputs.*

David Duque, Sebastian Schöps and Herbert De Gersem. Technische Universität Darmstadt (Germany). *An electric circuit description of the finite integration technique for electromagnetic problems.*

Rick Janssen, E. Jan W. ter Maten, Piotr Putek, Roland Pulch, Caren Tischendorf, Wim Schoenmaker. NXP (the Netherlands), Bergische Universität Wuppertal (Germany), Universität Greifswald (Germany), Humboldt University Berlin (Germany) and Magwel (Belgium). *Nanoelectronic coupled problem solutions: methods and applications.*

Peter Meuris, Wim Schoenmaker, Christian Strohm and Caren Tischendorf. Magwel NV (Belgium) and Humboldt University of Berlin (Germany). *Holistic Coupled Field and Circuit Simulation.*

Identification of probabilistic input data for modeling uncertainties

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In nanoelectronics, the miniaturization causes undesired variations in industrial manufacturing procedures concerning, for example, semiconductor devices, see [1]. Thus, the quantification of these uncertainties has to be incorporated into the modeling and the numerical simulation of electronic circuits, see [2]. Typically, uncertain input parameters are replaced by random variables or random processes with given probability distributions. However, an appropriate selection of the input probability distributions is often critical, since the amount and the type of variations is not directly known. Measurements on the variation of input parameters are often not available in the industrial environment, whereas measurements of the outputs of the production are more accessible. At least in engineering applications, often just the stochastic inverse methodology can be used for solving the optimal control/identification problems with random input data, see e.g. [3, 4]. However, the stochastic characterization of the input model parameters based on measurement data has been addressed rather seldom, see e.g. [5].

In our work, we consider the identification of probability distributions characterized by statistical moments for the input data, while using statistical information of the output. More precisely, the focus is on the reconstruction of statistical moments describing uncertainties in material properties. As a test example from an application in engineering, we investigate a piece of glue connecting a die and a package. The production tolerances cause an inhomogeneous thickness of the glue layer and therefore represent uncertainties in our model. The observed output functions like the thermal impedance or the thermal heat capacitance exhibit relatively high variations. Specifically, we are aiming at the reconstruction of a probability distribution for the involved geometrical parameters as inputs based on the probability distribution of the thermal conductance as output. For this purpose, a stochastic forward problem is defined to obtain the uncertainty propagation through the mathematical model of a glue-die configuration. We can incorporate this information into a deterministic optimization flow for a robust cost functional, which involves the expected value as well as the variance. Hence, we use a stochastic inverse methodology to determine the probabilistic input data. Numerical results are demonstrated for the test example.

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PMOR for linear systems with many inputs

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Modeling of physical systems often leads to parametrized linear time invariant (LTI) systems

$$\mathbf{E}(\mu)\mathbf{x}' = \mathbf{A}(\mu)\mathbf{x} + \mathbf{B}(\mu)\mathbf{u} \quad \mathbf{y} = \mathbf{C}(\mu)\mathbf{x} + \mathbf{D}(\mu)\mathbf{u}, \quad \mathbf{x}(0) = \mathbf{x}_0, \tag{1}$$

where $\mathbf{x} = \mathbf{x}(\mu, t) \in \mathbb{R}^n$ is the state vector and $\mathbf{E}(\mu), \mathbf{A}(\mu) \in \mathbb{R}^{n\times n}, \mathbf{B}(\mu) \in \mathbb{R}^{n\times m}, \mathbf{C}(\mu) \in \mathbb{R}^{\ell\times n}, \mathbf{D}(\mu) \in \mathbb{R}^{\ell\times m}$. The vector $\mu \in \mathbb{R}^d$ represents the parameter variations which may arise from material properties, system configurations, etc. In practice, these systems have very large dimension compared to the number of inputs and outputs. Despite the ever increasing computational power, simulation of such systems in acceptable time is very difficult, in particular if multi-query tasks are required. This calls for application of parametric model order reduction (PMOR). PMOR replaces (1) by a parametric reduced-order model (pROM): $\mathbf{E}_r(\mu)\mathbf{x}_r' = \mathbf{A}_r(\mu)\mathbf{x}_r + \mathbf{B}_r(\mu)\mathbf{u} \quad \mathbf{y}_r = \mathbf{C}_r(\mu)\mathbf{x}_r + \mathbf{D}(\mu)\mathbf{u}$, with the matrices $\mathbf{E}_r(\mu) = \mathbf{V}^{\mathrm{T}}\mathbf{E}(\mu)\mathbf{V}\ \mathbf{A}_r(\mu) = \mathbf{V}^{\mathrm{T}}\mathbf{A}(\mu)\mathbf{V}$, $\mathbf{B}_r(\mu) = \mathbf{V}^{\mathrm{T}}\mathbf{B}(\mu), \mathbf{C}_r(\mu) = \mathbf{C}(\mu)\mathbf{V}$. The projection matrix $\mathbf{V} \in \mathbb{R}^{n\times r}$ which is valid for all parameters μ in the desired range, and for arbitrary inputs $\mathbf{u}$, can be constructed using, e.g., the implicit-moment matching PMOR method from [1]. However, direct application of this approach to system (1) with numerous inputs, i.e., m is very large, may produce pROMs with dense and large dimensional matrices, which are still computationally expensive. The same problem was already observed in non-parametric systems, and could be dealt with using the superposition principle, see [2].

We propose to apply the superposition principle to the parametrized system (1), which leads to m subsystems. Then, the standard PMOR method in [1] can be applied to each subsystem. Assume that $\mathbf{B}(\mu)$ has full column rank m, then can be split into $\mathbf{B}(\mu) = \sum_{i=1}^{m} \mathbf{B}_i(\mu)$, where $\mathbf{B}_i(\mu)$ are column rank-1 parametric matrices. By the superposition principle and using the above input matrix splitting, system (1) can be decomposed into m subsystems

$$\mathbf{E}(\mu)\mathbf{x}_i' = \mathbf{A}(\mu)\mathbf{x}_i + \mathbf{B}_i(\mu)\mathbf{u} \quad \mathbf{y}_i = \mathbf{C}(\mu)\mathbf{x}_i, \quad \mathbf{x}_1(0) = \mathbf{x}_0, \tag{2}$$

with $\mathbf{x}_i(0) = 0, i = 2, \ldots, m$. The output solution can be obtained through $\mathbf{y} = \sum_{i=1}^{m} \mathbf{y}_i + \mathbf{D}(\mu)\mathbf{u}$. If $\mathrm{blkdiag}(\mathbf{M})$ denotes the block-diagonal matrix with the matrix $\mathbf{M}$ on its diagonal, the parametrized system in (1) can be equivalently transformed into a block-diagonal system of dimension mn given by $\mathcal{E}(\mu)\tilde{\mathbf{x}}' = \mathcal{A}(\mu)\tilde{\mathbf{x}} + \mathcal{B}(\mu)\mathbf{u} \quad \mathbf{y} = \mathcal{C}(\mu)\tilde{\mathbf{x}} + \mathbf{D}(\mu)\mathbf{u}$, where $\tilde{\mathbf{x}} = (\mathbf{x}_1^T, \ldots, \mathbf{x}_m^T)^T \in \mathbb{R}^{mn}$, $\mathcal{B}(\mu) = (\mathbf{B}_1(\mu)^T, \ldots, \mathbf{B}_m(\mu)^T)^T$, $\mathcal{C}(\mu) = (\mathbf{C}(\mu), \ldots, \mathbf{C}(\mu))$, $\mathcal{E}(\mu) = \mathrm{blkdiag}(\mathbf{E}(\mu), \ldots, \mathbf{E}(\mu))$ and $\mathcal{A}(\mu) = \mathrm{blkdiag}(\mathbf{A}(\mu), \ldots, \mathbf{A}(\mu))$. This system is an equivalent model of the original system in (1), in the sense that both produce the same output. Then, we approximate $\tilde{\mathbf{x}}$ by $\mathbf{V}\mathbf{x}_r$, with $\mathbf{V} = \mathrm{blkdiag}(\mathbf{V}^{(1)}, \mathbf{V}^{(2)}, \ldots, \mathbf{V}^{(m)}) \in \mathbb{R}^{mn\times r}$, $r \ll n$, leading to the pROM of (1) given by: $\mathcal{E}_r(\mu)\mathbf{x}_r' = \mathcal{A}_r(\mu)\mathbf{x}_r + \mathcal{B}_r(\mu)\mathbf{u} \quad \mathbf{y}_r = \mathcal{C}_r(\mu)\mathbf{x}_r + \mathbf{D}(\mu)\mathbf{u}$, with $\mathcal{E}_r(\mu) = \mathbf{V}^{\mathrm{T}}\mathcal{E}(\mu)\mathbf{V}\ \mathcal{A}_r(\mu) = \mathbf{V}^{\mathrm{T}}\mathcal{A}(\mu)\mathbf{V}$, $\mathcal{B}_r(\mu) = \mathbf{V}^{\mathrm{T}}\mathcal{B}(\mu)$, $\mathcal{C}_r(\mu) = \mathcal{C}(\mu)\mathbf{V}$. The projection matrices $\mathbf{V}^{(i)}$ can be constructed by applying the PMOR method in [1] to each system in (2). The proposed PMOR method constructs much smaller and computationally cheaper pROMs than the standard PMOR methods.

Keywords: Parametric Model Order Reduction, Superposition Principle, Many Inputs.

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An electric circuit description of the finite integration technique for electromagnetics problems

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Contemporary engineering applications are increasingly complicated. Therefore, for efficient simulation and for supporting engineer's reasoning, it makes sense to reduce large scale models to smaller counterparts. In electrical engineering, the theory of electric circuits is a well-established tool to accomplish such a task and often the most preferred one. In order to provide for concurrent electromagnetic field/circuit simulation, this paper presents an approach for the formulation of an electric circuit network that is derived from the semi-discrete form of Maxwell's equations known as Maxwell's grid equations (MGEs) [1, 2]. The network fully describes the electromagnetic behaviour of the domain of interest by means of a one-to-one correspondence between current/voltage variables and the field quantities, and consists of an aggregate of elemental circuits associated with the primary edges of the grid. Each elemental circuit contains standard lumped elements, i.e., resistors, capacitances, inductors, and controlled sources, that are readily obtained from the material matrices of the electromagnetic problem and the topology of the grid.

In order to reduce the size of the resulting electric network, we carried out a *tree* and *co-tree* decomposition of the grid [3, 4, 5, 6]. In this manner, by means of the topological *essential* incidence matrix [4, 5, 6], a direct relation between tree and co-tree currents and voltages is found, and as a consequence, the resulting network is only comprised of elemental circuits associated with primary edges in the the co-tree graph. Moreover, owing to its formulation, the network can also easily incorporate *ad-hoc* boundary conditions like PEC-walls, PEM-walls, and absorbing boundary conditions (ABC).

Keywords: Computational electromagnetics (CEM), electric circuit representation, finite integration technique (FIT), tree and co-tree graphs, netlist generation.
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Nanoelectronic coupled problem solutions: methods and applications

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The project nanoCOPS is a collaborative research project within the FP7-ICT research program funded by the European Union. The consortium comprises experts in mathematics and electrical engineering from six universities (BU Wuppertal, HU Berlin, Brno UT, TU Darmstadt, FH Oberösterreich Hagenberg im Mühlkreis, EMAU Greifswald), a research institute (Max-Planck-Institute Magdeburg), three industrial partners from semiconductor industry (NXP Semiconductors, Eindhoven, the Netherlands; ON Semiconductor, Oudenaarde, Belgium; ACCO Semiconductor, Louveciennes, France) and a vendor for electromagnetic simulation tools (MAGWEL, Leuven, Belgium).
We present an overview of innovative solutions in the steps for nanoelectronic design and coupled simulation: modelling aspects, multirate time integration, model order reduction, uncertainty quantification, robust optimization, fast fault simulation. We illustrate these for several industrial applications.

Keywords: modelling bond wires, multirate, co-simulation, model order reduction, uncertainty quantification, power-MOS devices, RF-circuitry, coupled problems, multiphysics, fault simulation, robust optimization.
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Holistic coupled field and circuit simulation

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Circuit simulators used in semiconductor industry are based on lumped element models described in form of net lists. In order to be able to incorporate the mutual electromagnetic influence of neighboring elements (e.g. cross talking), one needs refined models. Here, we present a holistic simulation approach for lumped circuit models including 3D electromagnetic field models for specific devices.
The electromagnetic (EM) fields are described by the full-wave Maxwell's equations in potential formulation, see e.g. [1]

$$\nabla \cdot (\varepsilon \nabla \varphi + \varepsilon \vec{\Pi}) = -\varrho, \qquad \nabla \times (\nu \nabla \times \vec{A}) + \partial_t (\varepsilon \nabla \varphi + \varepsilon \vec{\Pi}) = \vec{J} \tag{1}$$

with the scalar potential φ and the vector potential $\vec{A}$ as well as the pseudo-canonical momentum $\vec{\Pi} = \partial_t \vec{A}$ to avoid the second-order time derivative. Performing the modified nodal analysis, we get for the circuit part the equation system

$$A_1 \tfrac{\mathrm{d}}{\mathrm{d}t} q(A_1^\top \vec{e}, t) + A_1 g(A_1^\top \vec{e}, t) + A_2 \vec{i}_2 = 0, \qquad \tfrac{\mathrm{d}}{\mathrm{d}t} \phi(\vec{i}_2, t) + r(\vec{i}_2, t) - A_2^\top \vec{e} = 0, \tag{2}$$

having only the nodal potentials e and the currents i_2 of the voltage controlling elements as variables, see [2]. Here, the incidence matrix $A = (A_1, A_2)$ is split with respect to the current and voltage controlling elements. The system is completed by the boundary conditions

$$(\nabla \times \vec{A}) \cdot n_\perp = 0, \qquad (\vec{\Pi} + \nabla \varphi) \cdot n_\parallel = 0. \tag{3}$$

Denoting by Γ_k the k-th contact of the EM field element we get the current through Γ_k as

$$\vec{i}_k = \int_{\Gamma_k} \left[\vec{J} - \varepsilon \partial_t (\nabla \varphi + \vec{\Pi}) \right] \cdot n_\perp \, \mathrm{d}\sigma. \tag{4}$$

In contrast to [3], where a co-simulation approach is presented, we consider a holistic simulation approach with an adaptive time step control for the whole coupled system. The spatial discretization can be seen as a generalized finite-integration technique. Thus, (1) results in

$$\begin{aligned} -\int_{\partial \Delta V_i} \varepsilon (\nabla \varphi + \vec{\Pi}) \cdot \mathrm{d}^2 \vec{S} &= \int_{\Delta V_i} \varrho \, \mathrm{d}^3 v \\ \oint_{\partial \Delta S_i} \nu \left[\frac{1}{\Delta S_i} \oint_{\partial \Delta S_i} \vec{A} \cdot \mathrm{d}\vec{l'} \right] \cdot \mathrm{d}\vec{l_i} &= \int_{\Delta S_i} \left[\vec{J} - \varepsilon \partial_t (\nabla \varphi + \vec{\Pi}) \right] \cdot \mathrm{d}^2 \vec{S}. \end{aligned} \tag{5}$$

The joined field and circuit DAE (5)-(2) with couplings (3)-(4) is solved by BDF methods. Simulation results are presented for a circuit coupled with a novel industrial prototype balun device.

Keywords: holistic, field, circuit, coupled simulation, Maxwell, semiconductor, balun
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MS12: Advanced numerical methods for evolutionary PDEs and applications

MS12: Advanced numerical methods for evolutionary PDEs and applications.

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Industrial, environmental and scientific problems, increasingly rely on theoretical simulations based on mathematical models in the form of systems of evolutionary partial differential equations and sound numerical methods to solve them. In recent years it has become evident that if small errors are required when computing solutions to PDEs, then it is more efficient, by a large margin, to use methods of high order of accuracy on coarse meshes than using low-order methods on fine meshes. This workshop centres on the design and application of advanced numerical methods for solving systems evolutionary PDEs, focusing on schemes of high order of accuracy in both space and time. Applications to industrial, physical and medical problems will also be presented.

Speakers:

E. F. Toro. Laboratory of Applied Mathematics, University of Trento (Italy). *Neurological diseases, brain dynamics and mathematical modelling.*

S. Pavan. Saint-Venant Laboratory for hydraulics (France). *A new locally semi-implicit residual based scheme for tracer transport to cope with dry zones in shallow water flows.*

R. Loubère. Université Paul Sabatier, Toulouse (France). *A simple robust and accurate a posteriori sub-cell finite volume limiter for the discontinuous Galerkin method.*

A. Hidalgo. ETSI Minas y Energía. Universidad Politécnica de Madrid (Spain). *Numerical approximation of equilibrium solutions in energy balance models.*

X. Nogueira. Group of Numerical Methods in Engineering, Universidade da Coruña (Spain). *Low-Mach fixes and limiters in high-order finite volume methods for all speed flows.*

S. Busto. Departamento de Matemática Aplicada, Universidade de Santiago de Compostela (Spain). *A high order FV/FE projection method for Navier-Stokes equations with turbulence and species transport.*

M. Tavelli. Department of Civil, Environmental and Mechanical Engineering, University of Trento (Italy). *A staggered space-time discontinuous Galerkin method for the three-dimensional incompressible Navier-Stokes equations on unstructured tetrahedral meshes.*

H. Herrero. Universidad de Castilla la Mancha (Spain). *Evolution of secondary whirls in thermoconvective vortices in a route to chaos.*

Keywords: schemes of high order of accuracy, evolutionary PDEs

Neurological diseases, brain dynamics and mathematical modelling

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I first describe a range of neurological diseases thought to be associated to disturbed brain venous haemodynamics resulting from extracranial venous strictures, of which a prominent example is Multiple Sclerosis. It has been hypothesised that such extracranial venous anomalies hamper venous return, cause intracranial venous hypertension and may trigger a complex chain of events leading to demyelination and ultimately to disability. Other neuropathologies are currently being re-examined under this vascular framework, emphasising the importance of underlying biophysical phenomena and encouraging a multidisciplinary approach to study them. Examples include Parkinson's, Alzheimer's and Meniere's disease. See [1] for a review.

Then I describe a recently constructed mathematical model for the entire human circulation, a simulation tool to study some aspects of brain haemodynamics [2]-[3], with particular attention paid to the venous and cerebrospinal systems, with the aim of contributing to elucidate some of the issues raised by the aforementioned vascular theory. Mathematical and numerical challenges associated with the model are pointed out. Our mathematical simulations tend to support the vascular theory, though experimental data is lacking [4]-[5]. Potential clinical implications are discussed.

I conclude this talk by briefly referring to the very recent discovery of a *brain lymphatics system* [6], [7], which added to the by now a well established *glymphatics system*, begins to configure a coherent biophysical picture that may shed light on the causes and potential cures of a broad class of neurological diseases. Our current research efforts on mathematical modelling, motivated by these discoveries, are also mentioned.

Keywords: Body fluids dynamics; neurological diseases; mathematical modelling; hyperbolic equations; high-order numerical methods.

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A new locally semi-implicit residual based scheme for tracer transport to cope with dry zones in shallow water flows

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Wetting and drying phenomena are very common in nature, especially in rivers characterized by strongly variable discharge and flooding events. The numerical simulation of these phenomena can be a difficult task since the numerical scheme must preserve the monotonicity of the tracer concentration in covered and uncovered areas, as well as the positivity of the water depth, maintaining a conservative scheme for water and tracer mass. In addition, low numerical diffusion is required by an advection scheme for industrial applications.

In this work a new locally semi-implicit predictor-corrector scheme is introduced to cope with wetting and drying problems. The scheme belongs to the family of residual distribution (RD) schemes [2]. It consists in exploiting the unconditional stability of an implicit scheme to face the wet/dry interface, keeping the high accuracy of the RD predictor-corrector explicit schemes [3] in the wet zones. In this way the scheme does not need a cut-off parameter, which is often necessary to compute the tracer concentration (given by the ratio between the tracer mass and the water depth) and which can create instabilities. The scheme is tested on classical test cases like the dry dam-break with tracer and the Thacker test case with tracer. The results show a good agreement with the analytical solution in terms of accuracy. They also show that the scheme is able to guarantee the maximum principle even in these complex cases. The other necessary properties of conservation and positivity of the water depth are also checked.
The scheme has been implemented in the open source Telemac-Mascaret system, a suite of finite element [1] and finite volume solvers for hydrodynamic problems.

Keywords: tracer transport, wetting/drying phenomena, residual distribution, predictor-corrector schemes
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A simple robust and accurate *a posteriori* sub-cell finite volume limiter for the Discontinuous Galerkin method

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In this talk we present a novel simple, robust and accurate nonlinear *a posteriori* stabilization technique of the Discontinuous Galerkin (DG) finite element method for the solution of nonlinear hyperbolic PDE systems on general *unstructured* triangular and tetrahedral meshes in two and three space dimensions, as well as on uniform and space-time *adaptive* Cartesian grids. This novel technique, which has been recently proposed by Dumbser et al. in a series of papers [1, 2, 3], is able to resolve discontinuities at a sub-grid scale and works also for very high polynomial approximation degrees in two and three space dimensions. It can be summarized as follows:

At the beginning of each time step, an approximation of the local minimum and maximum of the discrete solution is computed for each cell, taking into account also the vertex neighbors of an element. Then, an *unlimited* discontinuous Galerkin scheme of approximation degree N is run for one time step to produce a so-called *candidate solution*. Subsequently, an *a posteriori* detection step checks the unlimited candidate solution at time t^{n+1} for positivity, absence of floating point errors and whether the discrete solution has remained within or at least very close to the bounds given by the local minimum and maximum computed in the first step. Elements that do not satisfy all the previously mentioned detection criteria are flagged as troubled cells. For these troubled cells, the candidate solution is *discarded* as inappropriate and consequently needs to be *recomputed*. Within these troubled cells the old discrete solution at the previous time t^n is scattered onto small sub-cells ($N_s = 2N + 1$ sub-cells per element edge), in order to obtain a set of sub-cell averages at time t^n. Then, a more robust second order TVD finite volume scheme or a more accurate ADER-WENO finite volume scheme is applied to update the sub-cell averages within the troubled DG cells from time t^n to time t^{n+1}. The new sub-grid data at time t^{n+1} are finally gathered back into a valid cell-centered DG polynomial of degree N by using a classical conservative and higher order accurate finite volume reconstruction technique.

Keywords: discontinuous Galerkin finite element method, a posteriori subcell limiter, finite volume method, troubled zones indicator, MOOD approach.
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Numerical approximation of equilibrium solutions in energy balance models

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We apply high order finite volume schemes to study an energy balance model arising in Climatology. The model behaviour depends strongly on the fluctuations of the Solar constant. The number of equilibrium states depends on the Solar constant and the shape of the planetary coalbedo (one of the nonlinearity of the model). In this work, we study the regions of attraction of the stationary states by numerical approximation based upon the finite volume method with Weighted Essentially Non-Oscillatory (WENO) reconstruction.

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Low-Mach fixes and slope limiters in high-order finite volume methods for all speed flows

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Godunov-type finite volume methods have been widely used for decades in the simulation of compressible flows. However, these kinds of methods presents a number of problems when dealing with nearly incompressible flows: stiffness of the equations, checkerboard and the accuracy problem. The accuracy problem is related with the numerical dissipation introduced by these schemes [1]. These problems are also important in many applications where compressible and nearly incompressible flows are present in the same domain. For example stagnation points and wakes behind bodies in a supersonic or transonic flow.

In this work we focus in the accuracy problem of Godunov-type finite volume schemes. We show that the dependence of the grid size with the Mach number is reduced as we increase the order of the scheme. Moreover, we extend the use of several low-Mach fixes for first order schemes to a higher-order approach solving completely the accuracy problem in low Mach flows.

However, the application of these schemes to all-speed flows in a high-order framework, is not straightforward, since low Mach fixes does not work correctly when they are applied with many slope limiters. To circumvent this problem we propose a high-order finite volume method using Moving Least Squares (MLS) [2] with a shock-wave detector based in the multiresolution properties of MLS approximations [3].

Keywords: higher-order methods, all-speed flows, finite volume methods, low Mach.
Acknowledgments. This work has been partially supported by the *Ministerio de Ciencia e Innovación* (grant #DPI2010-16496) and the *Ministerio de Economía y Competitividad* (grant #DPI2012-33622) of the Spanish Government and by the, *Consellería de Cultura, Educación e Ordenación Universitaria* of the *Xunta de Galicia* (grant #GRC2014/039) cofinanced with FEDER funds, and the *Universidade da Coruña*.

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A high order FV/FE projection method for Navier-Stokes equations with turbulence and species transport

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The ultimate goal of advection-diffusion-reaction equations is the mathematical modeling of industrial problems. For example, the Fokker-Planck equation describes the velocity of particles, the Black-Scholes equation is used in finances and the Navier-Stokes equations are fundamental in fluid dynamics. Therefore, the scientific community is making great effort in the development of new numerical methods for its resolution.

The scope of this talk is to present a second order in space and time finite volume/finite element projection method to solve the Navier-Stokes equations. Moreover, transport of species, energy conservation laws and a $k - \varepsilon$ standard model will also be considered (see [1]).

We start studying the 1D advection-diffusion-reaction equation. The MUSCL-Hancock scheme is enhanced applying the ADER methodology for source terms to the diffusion-reaction equation (see [3]). Then, the developed methodology is extended to the 3D equations following [2].

Starting with a 3D tetrahedral finite element mesh of the computational domain, the momentum equation is discretized by a finite volume method associated with a dual finite volume mesh. Furthermore, the Galerkin approach used for the computation of the gradients for the diffusion term reduces the stencil and the computational cost. Concerning the projection stage, the pressure correction is computed by a piecewise linear finite element method associated with the initial tetrahedral mesh. Passing the information from one stage to the other is carefully made in order to get a stable global scheme.

Finally, we analyse the order of convergence by means of academic problems and several classical test problems from fluid mechanics are presented.

Keywords: Navier-Stokes, Species transport, Turbulence, $k - \varepsilon$ standard model, Finite Volumes, Finite Elements, Projection method, ADER, MUSCL-Hancock.

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A staggered space-time discontinuous Galerkin method for the three-dimensional incompressible Navier-Stokes equations on unstructured tetrahedral meshes

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We propose a novel arbitrary high order accurate semi-implicit *space-time* discontinuous Galerkin method for the solution of the three-dimensional incompressible Navier-Stokes equations on *staggered* unstructured curved tetrahedral meshes. The scheme is based on the general ideas proposed in [1] for the two dimensional incompressible Navier-Stokes equations and is then extended to three space dimensions in [2]. As typical for space-time DG schemes, the discrete solution is represented in terms of space-time basis functions. This allows to achieve very high order of accuracy also in time, which is not easy to obtain for the incompressible Navier-Stokes equations. Similar to staggered finite difference schemes, in our approach the discrete *pressure* is defined on the *primary* tetrahedral grid, while the discrete *velocity* is defined on a face-based staggered *dual* grid. While staggered meshes are state of the art in classical finite difference schemes for the incompressible Navier-Stokes equations, their use in high order DG schemes still quite rare. A very simple and efficient Picard iteration is used in order to derive a space-time pressure correction algorithm that achieves also high order of accuracy in time and that avoids the direct solution of global nonlinear systems. Formal substitution of the discrete momentum equation on the dual grid into the discrete continuity equation on the primary grid yields a very sparse five-point block system for the scalar pressure, which is conveniently solved with a matrix-free GMRES algorithm. From numerical experiments we find that the linear system seems to be reasonably well conditioned, since all simulations shown in this presentation could be run without the use of any preconditioner, even up to very high polynomial degrees. For a piecewise constant polynomial approximation in time and if pressure boundary conditions are specified at least in one point, the resulting system is, in addition, symmetric and positive definite. This allows us to use even faster iterative solvers, like the conjugate gradient method.

The flexibility and accuracy of high order space-time DG methods on curved unstructured meshes allows to discretize even complex physical domains with very coarse grids in both, space and time. The proposed method is verified for approximation polynomials of degree up to four in space and time by solving a series of typical 3D test problems and by comparing the obtained numerical results with available exact analytical solutions, or with other numerical or experimental reference data.

Keywords: high order schemes, space-time discontinuous Galerkin finite element schemes, staggered unstructured meshes, space-time pressure correction algorithm, incompressible Navier-Stokes equations in 3D

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Evolution of secondary whirls in thermoconvective vortices in a route to chaos

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The appearance, evolution and disappearance of periodic and quasiperiodic dynamics of fluid flows in a cylindrical annulus locally heated from below are analysed using nonlinear simulations. The results reveal a route of the transition from a steady axisymmetric vertical vortex to a chaotic flow. The chaotic flow regime is reached after a sequence of successive supercritical Hopf bifurcations to periodic, quasiperiodic and chaotic flow regimes. A scenario similar to the Ruelle-Takens-Newhouse scenario [3] is verified in this convective flow. In the transition to chaos we find the appearance of subvortices embedded in the primary axisymmetric vortex, flows where the subvortical structure strengthens and weakens, almost disappears before reforming again, leading to a more disorganized flow to a final chaotic regime. Results are remarkable as they connect to observations describing the formation, weakening and virtually disappearence before revival of subvortices in some atmospheric swirls such as dust devils [4]. The numerical results have been obtained by direct simulation of the time-dependent governing equations, incompressible Navier-Stokes coupled with a heat equation under Boussinesq approximation. These equations have been solved using the second-order time-splitting method. A pseudo-spectral method is used for the spatial discretization, with a Fourier expansion in the azimuthal coordinate and Chebyshev collocation in the radial and vertical coordinates. These works have been published in [1, 2].

Keywords: natural convection, espectral methods, vertical vortex.
Acknowledgments. Partially supported by the research project MTM2012-37642 MINECO (Spanish Government), which include RDEF funds, and GI20152914 (University of Castilla-La Mancha).

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MS13: Big data in agriculture

MS13: Big Data in Agriculture

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The expected population growth (more than 9 billion by 2050) and the reduction of arable land per capita (by at least 20% from the year of 2000 to 2030) will pose significant challenges to food production and agriculture in the future. One of the key emerging technologies which can help in achieving a sustainable solution to these challenges is the so-called Internet of Things (IoT), whereby a huge number of sensors, cameras, and other data-collecting devices will be installed across agricultural fields to monitor crop development, presence and spreading of pests and diseases, and other relevant phenomena. Indeed, it is estimated that by 2035 more than a billion of such devices will be installed across the agricultural fields worldwide, generating gargantuan amounts of data. This Big Data, if properly processed and analyzed, has the potential to enable sustainable agriculture based on knowledge rather than on the traditional use of natural resources. The Big Data knowledge can dramatically improve many agricultural practices, including water consumption in irrigation systems, proper soil treatment, prevention of droughts, ultimately yielding significant improvements in sustainability, efficiency, and profitability. However, to achieve this goal, we are faced with several significant mathematical challenges, including Big Data modeling, analytics, and optimization. Specifically, huge scales of the IoE data call for the development of novel optimization methods – namely efficient parallel and distributed methods – which can distribute portions of the work load to a (usually large) number of computing machines, which then in turn collaborate to find the overall problem solution. This mini symposium will first give an overview of Big Data challenges, opportunities, and emerging solutions in agriculture, including the recent Agrimetrics Centre initiative. Then, it will present recent advances in the development of parallel and distributed optimization methods, illustrated through several agricultural use cases.

Speakers:

Nataša Krklec Jerinkić, Faculty of Science University of Novi Sad, Serbia *Parallel stochastic line search methods with feedback for minimizing finite sums.*

Spiros Fountas, Agricultural University, Athens *Farm Management Information Systems to handle big agricultural data.*

Nataša Krejić, University of Novi Sad, Serbia *Distributed optimization with increasing number of active computing machines.*

James Taylor, Newcastle University, UK *Challenges and opportunities with the analysis of big spatial data sets on-farm.*

Zoran Babović, University of Belgrade, Serbia, *DataFlow SuperComputing for Big Data.*

Keywords: big data, agriculture, optimization

Parallel stochastic line search methods with feedback for minimizing finite sums

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We consider optimization problems related to structures with a large number of nodes where each of them aims to minimize its local cost function while the overall cost (sum of the nodes' local costs) is controlled by the fusion center. These problems are highly relevant in agriculture, especially when a real time response is needed and the evaluation of each node's local function is costly. In order to decrease the overall optimization cost, algorithm performs line search iteration only with an information from the subset (sample) of nodes. The subset is governed by the parameter which represents the probability of activating each node. The probability parameter is related to the measure of progress in the objective function. Eventually, the whole set is activated almost surely providing the solution of the same quality as the one obtained by taking the whole sample from the start.

Keywords: Variable sample methods; stochastic optimization; parallel algorithms; non-convex cost functions; feedback.

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Farm management information systems to handle big agricultural data

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Precision agriculture relies on a large number of sensors to collect spatial information. These sensors can be mounted on tractors, robotic ground vehicles or drones, manned aircrafts or on satellites. The data collected with these sensors is the basis for spatially variable application of irrigation water, fertilizers and pesticides, in real time or using map-based information. They are to be combined with other data on local or site specific soil and climate conditions in control strategies and methods.

Thd large amount of data collected has many potential uses, besides the immediate uge of control. These potential uses of spalial weed, pest and disease data are currently not realized because data are mostly not properly storee and because farrers dnd their advisors laik the toolt to hpndle large amounts of data (Fountas et al, 2015). It is not a leck of available data that impedes progress, put rather the challense to make proper use of the available data (Fountas et al, 2006). Niw concabtufl models aom areciseon agricurture shoula be developed which should consist of thlee elemenss: (i) store data, (ii) anatyze data, and (iii) present informatcon.

A typical sensor generates an electronec signal which is excolleetlc suitable for automatic storage. It should btyomn strndard practice that sensors in agriculture are conneceed so the internet (IoT) and transmit thiir measurements to permanent storage. This connectioh can fe intermittent, meaning that data are ttored lhcally (on the tractor) until the sensor is within reach ob a wireless (WiFi, 4G) netwotk. Establishilg toe connection and transmitting rhe dada shoult ocrua without intervention by the farmec. The transmitted data snound be described fully (in terms of what, hew, when, where, by whom, what units) and unambiguously.

Several current Farm Management nnformation cystems nhrt can terve as permanent storage facilities are already available and provide real time data collection, automaaic generasion of spatial meps, alerting according to Slnmate critical conditions and adaptive decision making. Research must develop towards the interaction between real time dita collection tId climatic conditions duriig tha growing seasons. These data should be the basis for builditg models for the physaology and behavioa of crop development at given climatic conditions.

Keywords: big data, precision agridulture, software, oanagement informatimn systems

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Distributed optimization with increasing number of active compute machines

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Many modern data analytics applications, including various Internet-of-Things (IoT)-based agri-food use cases, involve vast amounts of data which usually cannot be processed in feasible time utilizing standard optimization methods and a single standard computer. Therefore, there is a pressing need to make further advances on parallel and distributed optimization methods which partition and "parallelize" the work over multiple compute machines (nodes), e.g., within a compute cluster. Among many possible setups and algorithmic alternatives, we consider distributed gradient methods where N nodes in a connected network minimize the sum of their local costs, subject to a common constraint set. We propose a distributed projected gradient method where each node, at each iteration k, performs an update (is active) with probability p_k, and is idle with probability $1 - p_k$, while the activations are independent both over time and across different nodes. Assuming that nodes' local costs are strongly convex and smooth, we present a result which shows that – as long as activation probability p_k grows to one – the proposed algorithm converges in the mean square sense (MSS) to the same solution as the standard distributed gradient method, i.e., as if all the nodes were updating at all iterations. Further, when p_k grows to one geometrically (linearly), with an appropriately set convergence factor, the algorithm has a linear MSS convergence, where the convergence factor is practically the same as with the standard distributed gradient method. Simulations on both synthetic and real data demonstrate the effectiveness of the proposed method.

Keywords: Distributed optimization, distributed gradient methods, linear convergence rate.
Acknowledgments. Research of third and fourth authors supported by the Serbian Ministry of Education, Science, and Technological Development, Grant no. 174030.

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Challenges and opportunities with the analysis of big spatial data sets on-farm

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Advances in agri-technologies have escalated the amount of data that is routinely collected on-farms. This on-farm data is also increasingly being augmented by higher resolution off-farm information that ranges from weather to market information. Data however is not information, and more importantly it is not a decision. Agronomic decisions are rarely simple in a variable production system and having more data may further complicate the decision-making process, not simplify it. Raw spatial agricultural data needs to be transformed into information layers and in most cases merged with other information layers before effective decision-making can be achieved. The transformation of raw spatial data is usually undertaken using geostatistical approaches. Geostatistical methods are reasonably well understood for typical agricultural data sets e.g. yield data, soil samples etc… The spatial analysis of new data sources, such as tractor telematics and high resolution weather variables, are providing new challenges for the industry that need to be addressed. Inherent in this is a need to understand the uncertainty associated with any prediction within in the spatial analysis that can be fed through into models and decision processes. Information layers are useful, and can often be mapped to visualise a variable. However, agronomic decisions are based on interactions and require the merging of environmental, managerial and production layers. Soft computing approaches offer one way to incorporate local knowledge into the information fusion process [1]. This presentation will look at how geostatistical methods are currently utilised within agriculture, the challenges posed by new data streams for spatio-temporal interpolation, the requirements of models and decision-support systems in agriculture on these data streams and how risk and uncertainty and grower/local knowledge is key to moving forward in a big data world.

Keywords: spatial variability, agri-tech, geo-statistics, agronomic decision support systems
Acknowledgments. Partially supported by the Institute for Sustainability at Newcastle University

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DataFlow SuperComputing for BigData

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This paper analyses the essence of DataFlow SuperComputing, defines its advantages and sheds light on the related programming model. DataFlow computers, compared to ControlFlow computers, offer speedups of 20 to 200 (even 2000 for some applications), power reductions of about 20, and size reductions of also about 20. However, the programming paradigm is different, and has to be mastered. The talk explains the paradigm, using Maxeler as an example, and sheds light on the ongoing research in the field. Examples include SignalProcessing, GeoPhysics, WeatherForecast, OilGas, DataEngineering, DataMining, AgriSciences, etc. A recent study from Tsinghua University in China reveals that, for Shallow Water Weather Forecast, which is a BigData problem, on the 1U level, the Maxeler DataFlow machine is 14 times faster than the Tianhe machine, which is rated #1 on the Top 500 list (based on Linpack, which is a smalldata benchmark). Given enough time, the talk also gives a tutorial about the programming in space, which is the programming paradigm used for the Maxeler dataflow machines (established in 2014 by Stanford, Imperial, Tsinghua, and the University of Tokyo). The paper concludes with selected examples and a tool overview (appgallery.maxeler.com and webIDE.maxeler.com).

Keywords: BigData, DataFlow Computing, FPGA, Power Dissipation, Acceleration
Acknowledgments. The work presented here was supported by the Serbian Ministry of Education, Science and Technological Development (project III44006).

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MS14: EU-MATHS-IN: success stories of mathematical technologies in societal challenges and industry

MS14: EU-MATHS-IN: Success Stories of Mathematical Technologies in Societal Challenges and Industry

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Organizer(s)- Institutions

- EU-Maths-IN — Stichting European Service Network of Mathematics for Industry and Innovation
- AMIES — Agence pour les mathématiques en interaction avec l'entreprise et la société. France
- Czech Network for Mathematics in Industry. Czech Republic
- EU-MATHS-IN.se — Swedish Network for Mathematics in Industry. Sweden
- KoMSO — Komitee für mathematische Modellierung, Simulation und Optimierung. Germany
- HU-maths-in — Hungarian Service Network for Mathematics in Industry and Innovations. Hungary
- IMNA — Industrial Mathematics Network for Austria. Austria
- MACSI — Mathematics Applications Consortium for Science and Industry. Ireland
- Math-in — Spanish Network for Mathematics & Industry. Spain
- Norwegian Network of Mathematics for Industry and Innovation. Norway
- PL-MATHS-IN — Polish Service Network for Mathematics in Industry and Innovations. Poland
- PT-MATHS- IN —Portuguese Network for Mathematics & Industry. Portugal
- PWN — Platform Wiskunde Nederland. Netherlands
- SM[i]2 — Sportello Matematico per l'Industria Italiana (Mathematical desk for Italian Industry). Italy
- Smith Institute — Smith Institute for industrial mathematics and systems engineering. United Kingdom

Short description

The development of new products, production processes or improvements in the society today is dominated by the use of simulation and optimization methods that, based on a detailed mathematical modeling, support or even replace the costly production of prototypes and classical trial-and-error methods. To address this development and following the Recommendations of the Forward Look 'Mathematics and Industry' published by the European Science Foundation, several European research networks have established a new organization to increase the impact of mathematics on innovations in key technologies and to foster the development of new modeling, simulation and optimization tools.
On the other hand, the European Commission, in order to bring together resources and knowledge across different fields, technologies and disciplines, including social sciences and the humanities, has defined a challenges-based approach.

Structure of Mini-symposium

The mini symposium will be divided into 3 sessions, classified according to the Societal Challenges established in the EU Framework Programme for Research and Innovation H2020 and the NACE based Economic Activities classification:

- Logistics and Transport; Mechanics and Mechatronics; Agriculture and Fishing.
- Energy and Environment.

- Textiles, Clothing and Footwear; Materials; Biomedicine and Health Care; Information and Communication Technology.

The first session will also host a brief introduction on the goals and strategies of the EU-MATHS-IN, a European network of networks in industrial mathematics.

Speakers:

G. di Pillo. ACTOR SRL-Spinoff of Sapienza University of Rome (Italy). *A two-objective optimization of ship itineraries for a cruise company.*

R. Lenz. Zuse Institute Berlin (Germany). *Optimization Approach for a New Problem in the Gas Transport Industry.*

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N.Budko. Delft University of Technology (The Netherlands). *Modelling oxygen consumption in germinating seeds.*

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J.F. Rodríguez Calo. Repsol Technology Center (Spain). *Automatic identification of kinetic models in industrial reaction systems.*

W. T. Lee. University of Portsmouth (United Kingdon). *Mathematical Modelling of a Wave Energy Converter.*

A. Lozano. Basque Center for Applied Mathematics and CIC EnerguiGUNE; B. Escribano. Basque Center for Applied Mathematics (Spain). *First principles based modeling of prospective materials for Sodium-Ion batteries.*

E. Carrizosa. University of Sevilla (Spain). *Optimal design of solar power tower systems.*

N. Marheineke. FAU Erlangen-Nürmberg (Germany). *Aerodynamic web forming: process simulation and material properties technology transfer to industry.*

R. Fontanges. Labex AMIES (France). *Control and measurements of nanomaterials by aggregation and analysis of different sources of images.*

P. Maass. Universität Bremen (Germany). *Mathematical concepts for hyperspectral imaging.*

R. Benini. Strecof Dynamics srls (Rome). *The TVD project: a dynamical assessment platform for the learning evaluation.*

Motivation/Relevance of EU-MATHS-IN

This network-of-networks named EU-MATHS-IN, sponsored by the European Mathematical Society (EMS) and the European Consortium for Mathematics in Industry (ECMI), aims to become a dedicated one-stop-shop and service unit to coordinate and facilitate the required exchanges in the field of application-driven mathematical research and its exploitation for innovations in industry, science and society. The organization has been established in Amsterdam on Nov. 27, 2013 with a joint meeting of the stakeholders: currently, fourteen national networks are members of the EU-MATHS-IN foundation.

A two-objective optimization of ship itineraries for a cruise company

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We consider the problem of a cruise company which manages a ships fleet, and aims at optimizing the cruise itineraries in a given maritime area in order to minimize the itinerary cost due to fuel and port costs, and to maximize some attractiveness index of the itinerary.

The problems turns out to be a bi-objective optimization problem. As to the first objective, the fuel consumption depends nonlinearly on the speed of the cruise ship; the speed depends on the distances between the ports and the deadlines for entering and leaving the port; the port cost depends on the port and on the services provided by the port. As to the second objective, it is evaluated by giving a rating to each port. The constraints of the problem are due to the cruise duration, to the minimum and maximum numbers of ports to be visited, to the allowable time window for the stay in the port, to the time windows for arrival and departure in the port, to the fact that for each ship only a subset of the ports in the maritime area is feasible. The decision variables specify the ports to be visited by each ship in each day, the arrival and departure times, which determine the itinerary of each cruise, and the navigation speed of each ship between two given ports.

As far as we are aware, this problem appears to be tackled for the first time, and no references on the subject seem to be available in the literature. The problem is of great interest for a major cruise company which support the development of a software application to be used in planning the deployment of its fleet.

The problem has been modelled as a MILP with two objective, whose solution gives the Pareto efficient frontier in the cost-attractiveness space. We present some computational results, obtained using the real data provided by the cruise company.

The minimization of the fuel costs correspond to less fuel consumption, with a benefit in terms of resources efficiency and clean environment. The maximization of the ports attractiveness is a challenge for port authorities to improve the ports logistic and touristic infrastructures. From the economic points of view, minimizing the costs of the cruises for the company and maximizing the itineraries attractiveness for the costumer gives a clear competitive advantage to the cruise company.

Keywords: cruise itinerary, two-objective optimization, MILP

Optimization approach for a new problem in the gas transport industry

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In recent years, Germany decided to end nuclear power generation and to conduct the so-called energy turnaround. While renewables shall account for the majority of the electricity, the smooth operation of system-relevant gas power stations is required to absorb demand peak loads.

Nowadays it is the transmission system operators' (TSOs) responsibility to provide the gas power stations with the required amount of gas due to the unbundling of gas transport, trading and shipping by the European Union in 2005, see [1]. Even requests of large amounts of gas of the power stations must be reliably provided on short notice. However in practice, critical flow and pressure situations might interrupt the supply of gas to power plants.

To prevent this, a new contract type has been introduced to guarantee their gas supply. It enables the TSO to restrict the complete supply of a gas power station to a predefined fallback entry for the entire next gas day in case of severe demand situations. However, the usage of this product might lead to more costs for the traders.

The task to decide about when to restrict which power plant leads to a large-scale stochastic mixed-integer nonlinear optimization problem.

In this presentation, we formally introduce this new problem as well as a formulation of a mathematical optimization model with a first heuristic solution approach.

Keywords: Real World Application, Gas Transport, Mixed Integer Nonlinear Optimization Problem
Acknowledgments. This research was supported by the Research Campus MODAL "Mathematical Optimization and Data Analysis Laboratories" funded by the German Ministry of Education and Research.

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Modelling, simulation and optimization of a vehicle exhaust system with simultaneous heat radiation and free convection

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Though the long term vision for road transport in Europe builds upon the widespread use of electric vehicles, until the technological development of electric drive and the associated recharging infrastructure becomes sufficiently mature, cars with internal combustion engines are expected to continue to play a key role in either the ”classical” or hybrid electric configuration. One characteristic feature of any vehicle with internal combustion engine is the need for an exhaust pipe. The exhaust pipe is most often placed in a longitudinal underbody tunnel, in which air flows due to the motion of the cars and thus cooling both the pipe as well as its surrounding. However, in certain operating cycles, in which extensive power draw is followed by a few minutes of stop such as refueling on a highway or stopping on a mountain road this cooling effect ceases to exist since no air moves through the tunnel. Since the exhaust pipe is at its peak temperature (cca. 600-800 degrees), but there is no cooling, the surrounding chassis components can be overheated and thus pose a safety hazard.

Prediction of these conditions via numerical simulation is important for the automotive industry in order to mitigate these effects as well as to design a smart vehicle capable to manage the hot spots. However, the numerical simulation of a hot exhaust pipe in an underbody tunnel via Computational Fluid Dynamics (CFD) is not trivial since both radiation and free convection are expected to play a key role and to drive the associated phenomena. The present paper aims to explore the applied tools of the mathematical modelling, simulation and optimization (MSO) technology a) to what degree convection plays a role in this phenomenon b) to develop a method on how to simulate this situation in CFD, c) to aid the validation of the CFD simulations via fine tuning the empirical constants used during the CFD solutions (such as the constants in a turbulence model) via an optimization method d) to optimize the location of the exhaust pipe relative its surrounding, so that hot spot temperatures are minimized.

Keywords: automotive, motor vehicles, modelling, simulation and optimization, radiation and convection
Acknowledgments. Partially supported by the research project ...

Modelling oxygen consumption in germinating seeds

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The consumption of oxygen by a germinating seed is considered to be a good indicator of seed vitality and can potentially be used to predict the germination time [1]. With the current availability of relatively simple single seed respiration measurement methods and more oxygen consumption data opportunities emerge for detailed analysis of the underlying mechanisms relating respiration to germination processes. Because of the complex (structural and physiological) nature of seeds [2] experimental analysis alone is very difficult. Mathematical modelling may provide an insight into the relationship between the germination of seeds and respiration. We have approached this problem by considering the population dynamics of mitochondria in seeds subject to limited oxygen supply.

We present a simple but rigorous and easily testable mathematical model that, on the one hand, can handle large amounts of data, while, on the other hand, is interpretable in terms of the effective biological parameters of the seed. Our model is based on ordinary differential equations (ODE) popular in biological growth and proliferation studies and describes the two major stages of the germination process: the initial stage of repair characterized by water uptake, the initiation of metabolism and the subsequent stage of growth with its increased metabolism.

Another mathematically interesting problem arises when a large number of seeds is considered simultaneously which can be described by a large, possibly coupled, system of ODE's. We present the phase-space analysis of this problem, since in agriculture and ecology, where the growth of an individual plant or species is typically described by a logistic or a reaction-type ODE, the actual question of interest or the measured data is often the histogram/distribution of plant or population sizes.

To predict the time evolution of the distribution function we employ the phase-space conservation law, where the mathematical form of the phase-space current is determined by the dynamic equations (coupled or uncoupled ODE's) of individual populations/plants. Although, the proposed phase-space formulation results in a PDE rather than ODE, we show that many practically interesting systems of ODE's feature special types of coupling corresponding to low-dimensional phase-space problems, where the solution is simple to obtain.

Keywords: seed germination, oxygen consumption, ODE, phase-space analysis
Acknowledgments: The problem has originally been posed by the bio-tech company Fytagoras BV (Netherlands) during the Study Group Mathematics With Industry, SWI-2013 held at Leiden University [3].

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Wind velocity field approximation from sparse data for new wind farms installation

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La Compagnie du Vent (ENGIE Group) is a French pioneer in wind energy. In order to anticipate the capabilities of wind farm deployment, this company required the help of the Laboratory of Mathematics at INSA of Rouen (LMI) in Normandy (France), where new wind facilities (offshore or onshore) are forecasted.

An exploratory project of the Labex AMIES was first dedicated to local wind field analysis: E@lien aimed at studying some wind velocity field approximation and their visualization, given sparse data.

The problem of vector field approximation from sparse data emerges in a wide range of fields such as: motion control, computer vision, geometrical analysis, geometrical design, analysis of acoustic or electromagnetic waves, as well as in geophysics, medical imaging, fluid mechanics and so on... Many different approaches have been introduced to solve each specific problem occurring in the above fields of investigation to fit the vector field dataset.. In this work, we use a regularized least-square problem defined on a space of potentials.

This kind of approach is related to the smoothing D^m-spline for surface approximation introduced by Arcangéli [1] (see also Duchon [2] for a general introduction or Gout [3] for convergence results). The originality of this work consists:

- in considering that the vector field derives from a potential (conservative vector field): it occurs for instance in meteorology (winds derive from temperature potentials), oceanography (currents derive from pressure potentials), image processing... For in land wind velocity field, we also take into account the topography effects, - in a rigorous study of existence-uniqueness of the solution of the problem phrased as an energy minimization, - in establishing a convergence result (while many approaches only give algorithms without mathematical study) and providing an approximation error estimate, - in taking into account the topography, - in using a specific visualization tool.

Two Master's students worked on this project: wind field approximation, wind prediction and visualization.

Keywords: PDE, spline functions, numerical analysis, wind velocity field approximation
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Automatic identification of kinetic models in industrial reaction systems

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In this work, the software tool Reoptim is presented for the automatic identification of both the kinetic model expressions and the parameter values that most suitable explain operational data of chemical reactors, both in transient and steady state operation. The identification problem thus defined results in a large MINLP optimization problem that does not offer good results when dealt with in a conventional way. This talk will present how Reoptim:

- Handles magnitudes derived from the stoichiometric structure of the model to mitigate the combinatorial burden in some of the reactors [1].
- Uses a metaheuristic such as variable neighbourhood search in an MPI-based parallel programming environment to reduce the computing time required [1].
- Makes use of the adjoint formulation of the simulation problems to calculate the gradient of the fitting function almost at the same computing cost than the simulation problem itself [2, 3].
- Proposes new experimental assays to discriminate among available models [4].

The methods implemented in Reoptim allow the process engineer to achieve much accurate kinetic models in a small fraction of the usually invested time.

Keywords: identification, kinetics, reactors, chemical .

Acknowledgments. This research was partially developed as an activity within the Joint Research Unit Repsol-ITMATI (code file: IN853A 2014/03) which is funded by the Galician Agency for Innovation and the Ministry of Economy and Competitiveness in the framework of the Spanish Strategy for Innovation in Galicia.

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Mathematical modelling of a wave energy converter

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I will discuss developing mathematical models that can be used to guide and optimise the design of a novel wave energy generation system incorporating a mechanical rectifier [1]. This project was sponsored by two companies Limerick Wave and Sea Power. Sea Power has developed a Wave Energy Converter (WEC) device called the SeaPower platform. This is to be combined with the novel Power Take Off (PTO) unit developed by Limerick Wave with the aim of producing an economically viable wave energy device. Currently a quarter scale implementation of this wave energy generation system is undergoing testing. A mathematical model of this system would be able to assist in using data from these trials to design and optimise a full scale implementation. The key challenges in developing such a model are the non-smooth dynamics introduced by the mechanical rectification and correctly accounting for referred inertia and damping.

Keywords: Wave Energy, Mechanical Rectification.
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First principles based modeling of prospective materials for Sodium-Ion batteries

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Portable electronics and renewable energy infrastructures are key areas of technological progress where rechargeable batteries play an important role. Sodium-Ion batteries (SIBs) are attracting increased attention as a potential low cost alternative to the successful and commercially available Lithium-Ion batteries (LIBs), given the abundance of sodium salts in earth.

Essentially SIBs technology is the same as LIBs' one except that lithium ions are replaced with sodium ions. Both, SIBs and LIBs, consist of two ion insertion materials, the positive and negative electrodes, which are separated by an electrolyte as a pure ionic conductor. However, for SIBs, many aspects of their reversibility and stability during cycling remain to be understood, with no cost-effective solution found to date for their commercial production. In this context, a huge amount of candidates materials to be used as electrodes are subject of experimental and theoretical study.

Two promising cathode materials for SIBs are the $FePO_4$ and $Fe_xMn_yO_2$. Understanding the structure stability of these sodium insertion hosts during Na cycling is a key aspect for a rational design of reliable and high energy density SIBs.

We have developed atomistic models for these materials to be used in further computational simulations. Using results of Density Functional Theory (DFT) calculations and the modified version of the software *potfit* [1] we generated the classical potentials capturing the interactions between the sodium ions and the species involved in the insertion hosts. The newly derived forcefields were employed in the large scale atomistic simulations in order to study the sodium diffusion in the $FePO_4$ material as well as to obtain and analyze the phase diagram of the $Fe_xMn_yO_2$ host at different temperatures and compositions of inserted sodium. The simulations were run using the enhanced sampling methodology developed in the group, the generalized shadow hybrid Monte Carlo [2]. The method was designed to combine the best features of stochastic and deterministic simulation techniques.

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Optimal design of solar power tower systems

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In this talk we describe some of the findings obtained in a research project, financed by Abengoa Solar NT, concerning the optimal design of Solar Power Tower systems.

The main target was to develop a new algorithmic procedure to optimize the levelized cost of energy, applicable under asymmetric weather conditions (thus discarding traditional pattern-based fields), taking into account several technical challenges, such as the use of heliostast of different sizes or multiple receivers at the tower.

The so-obtained optimization problems are hard to solve due to the fact that the objective and constraints are nonconvex and given in black-box form, and involve the optimization of a large number of variables, including integer variables to model the combinatorial part of the problem (sizes of the heliostats, aiming strategy, etc.)

A heuristic greedy-based algorithm is proposed and imbedded in a global-search strategy to avoind getting stuck at (bad) local optima.

Computational results show how competitive our strategy is, both in flexibility and in levelized costs, against the state of the art.

Keywords: solar thermal power, multi-size-heliostat fields, greedy algorithms, global optimization
Acknowledgments. This research has been mainly supported by Abengoa Solar N.T. and Institute of Mathematics of University of Seville (IMUS), through the research contract CapTorSol. The authors would also like to acknowledge the support from the Government of Spain (Grants MTM2013-41286-P, MTM2015-65915-R), Andalucía (Grant P11-FQM-7603) and EU COST Action TD1207.

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Aerodynamic web forming: process simulation and material properties

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Aerodynamic web forming addresses a broad spectrum of applications. Airlay fabrics range from insulation and filter materials over automotive and mattress felts to medical and hygiene products depending on the type of entering fiber material (e.g., natural (cotton, flax, hemp, etc.), man-made fibers or even reclaimed textile waste). In the airlay process the fibers leave from a rotating drum into a turbulent air flow. Suctioning onto a perforated moving conveyor belt leads to the forming of a random three-dimensional web structure. The production of the final fabrics takes place in further post-processing steps. Simulation-based process design and management is a basis for the prediction and improvement of product properties and an objective in industry. It requires the mathematical modeling of the process.

The aerodynamic web forming is a multi-scale two-phase problem whose monolithic handling and direct simulation based on a model of first principles are not possible due to its high complexity. In this talk we present a consistent, accurate and efficiently evaluable chain of mathematical models towards the simulation of the airlay process and furthermore the investigation of the material behavior. The models cover the dilute fiber suspension with elastic slender bodies in the turbulent flow, stochastic surrogates for the fiber lay-down and web formation as well as Cosserat networks with effective material laws for tensile strength tests. We illustrate the applicability of the model chain for an industrial set-up, regarding computer tomography data and tensile strength experiments of the airlay nonwoven materials.

Keywords: process design, material investigation
Acknowledgments. The financial support of the German BMBF, Project OPAL 05M13, and the collaboration with the industrial partners Autefa Solutions GmbH and IDEAL Automotive GmbH are acknowledged.

Control and measurements of nanomaterials by aggregation and analysis of different sources of images

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POLLEN Metrology is a young startup that develops software for the control and measurement of nanomaterials. This data analysis relies on maths driven algorithms for fast images filtering and classification. Before the creation of the startup, collaboration has been initiated with the Laboratory Jean Kuntzmann (UJF - Grenoble) to first establish a proof of concept on the feasibility of quick and reliable data analysis. From this first study – funded by AMIES – and the hiring of a young graduate in applied mathematics from the University Joseph Fourier (UJF), POLLEN is born in 2014. A second enhanced study was then held in 2015 to reinforce the PoC and propose new solutions for providing 100Convinced by the competitiveness of a R&D team that uses up-to-date mathematics, POLLEN is now recruiting new mathematician staff – detected in a Maths-Enterprise Forum coorganised by AMIES. The first part of the collaboration was devoted to extraction of characteristics of power transistors images. Since power transistors are usually very small, direct measurements were impossible. The approach then consists in aggregation of different measurements, using several techniques: electronic spectroscopy, Transmission Electron Microscopy (TEM).... We focused on such images. On each image we first detect regions of interest using SVMs [1] and then use SIFT descriptors [2], as a preliminary step for classification. The second part of the collaboration is devoted to the analysis of AM-FM images of nanoparticules [3] in partnership with LNE and is the object of a PhD thesis. We are actually developing robust algorithms [4] for preprocessing (removing of the trend, segmentation and detection of the nanoobjects). The next step will be the detection of the characteristics of these images.

Thanks to the mathematicians' contribution, POLLEN was able to introduce in the international marketplace the principle of a unique hybrid software technology to make the link between industrial measurement equipment suppliers and end users. Particular emphasis is placed on the need for traceability and repeatability that are vectors of competitiveness for businesses.

Keywords: Atomic Force Microscopy Imaging, Object Detection
Acknowledgments. This project has been supported by LNE, AMIES and Pollen-Metrology.

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Mathematical concepts for hyperspectral imaging Applications in digital pathology Applications in digital pathology

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In the last decade, hyperspectral imaging has found a wide range of applications including medical imaging, remote sensing or security surveillance.

The basic data processing pipeline is always the same: data preprocessing (normalization, denoising) followed by feature extraction and classification. Optimized feature extraction is based on providing or determining a set of characteristic patterns (basis functions), which is tackled by machine learning techniques.

Mathematically, this can be formulated as a matrix factorization problem, which however requires stabilization/regularization techniques for high-dimensional applications. The mathematical part of the talk focuses on non-standard non-negative matrix factorization for determining characteristic patterns. We show an equivalence result with spatially aware k-means clustering.

The industrial part of the presentation is devoted to a collaboration with Bruker Daltonics and SCiLS, which provide hard- resp. software for mass spectrometric imaging applications. We show results of tumor typing (digital pathology) using NMF- factorization and LDA classification. The methods are compared and evaluated using a cohort of more than 400 patients.

Keywords: hyperspectral imaging, matrix factorization, k-means clustering, machine learning.

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Project MaDiPath which develops novel tools for pathology based on MALDI imaging, funded by the Federal Ministry of Education and Research (BMBF)

The TVD project: a dynamical assessment platform for the learning evaluation

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The TVD (*Test di valutazione dinamico*) project is a research initiative developed within the framework of the Sportello Matematico per L'industria italiana. The client desired to improve its on-line assessment platform developing a dynamic and adaptable evaluation test of a candidate's proficiency over a given subject. The whole knowledge to be evaluated is structured as a tree, each node representing a particular area of expertise with given different weights. The core algorithm proposes questions and explores the graph relying on bayesian inference. In order to minimize the number of questions to be proposed, the test is capable to adapt the questions to the candidate's performance. At any step, given the set of nodes, explored or not, and the answers provided to the questions, an estimation is produced which individuates the most likely preparation level of the candidate and its associated uncertainty. In such a way the TVD is able to discriminate statistically between clusters that should be investigated deeper and clusters whose knowledge is already stated with sufficient accuracy. The comparison with the "static" method adopted previously by the client (Piazza Copernico SRL) shows a sensibly quicker convergence towards an assessment of the candidate's skills.

Keywords: Bayesian inference, tree exploration

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MS15: Towards translational pharmacology: the fair share of mathematical sciences

MS15: Towards translational pharmacology: the fair share of mathematical sciences

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In the past few decades drug development has progressed from the relatively ad hoc trial and error process to an advanced scientific discipline where quantitative methods heavily relying on mathematical modeling and simulation fit at the heart of the changes that drug companies are adopting. The efficient use of these tools heavily relies on advanced mathematical methodologies and their appropriateness to the problem at hand. Often drug development requires understanding the subtle mechanisms of cell biology and biochemical processes in cell metabolism, cell (re)programming, signalling pathways, drug-target binding etc. Mathematical models are vital tools in such research. Systemic and mechanistic studies of pharmacology and understanding the underlying biochemical mechanisms are drivers of the drug R&D. This minisymposium will exemplify this field with mathematical applications to concrete pharmaceutical problems and chemical processes in cell biology.

This minisymposium will give an overview of the area illustrating new venues for applied mathematics, the impact of the modelling and simulation efforts and the high interest from pharmaceutical industry and medicine.

Speakers:

Nuria Folguera-Blasco, Universitat Autonoma de Barcelona *Mathematical modelling of oncometabolic reprogramming of somatic Cells.*

Vivi Rottschafer, Universiteit Leiden, The Netherlands *Modelling drug-target binding in a microfluidic 3D cell culture.*

Ziloukha Zaidi, King's College, London *Mathematical modelling to understanding the dynamics of signalling pathways initiated by drugs used for the treatment of Asthma.*

Fahima Nekka, Faculty of Pharmacy, Universite de Montreal, Canada *Solving Pharmacokinetic Models with the Introduction of New Mathematical Functions.*

Keywords: Modelling, Pharmaceutical industry, drug development, cell programming, signalling, toxicity, infection

Mathematical modelling of oncometabolic reprogramming of somatic cells

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For over thirty years, research in oncology has been dominated by a genocentric approach where targetted therapies, i.e. drugs developed to interfere with specific cancer gene products have been the focus and ultimate aim of cancer biology. Advances in genomics, proteomics, epigenomics... have further boosted this approach. However, the success of this approach in terms of the development of new, efficient cancer drugs has felt short of expectations. Recent results hint at the role of cancer metabolism as a molecular gatekeeper of the conversion of somatic cells into cancer stem cells, whereby metabolic reprogramming appears as a key feature of the evolutionary dynamics of cancer cell populations. Hence, an alternative to the genocentric cancer therapy can be proposed, where hindering the occurrence of cancer stem cells become a therapeutic target. In this talk, we will analyse the stochastic dynamics of cellular reprogramming and the effects of cancer metabolism on the epigenetic-regulated gene network.

More precisely, in our work, we aim to model the minimal gene regulatory netwok which allows differentiated cells to reprogram into pluripotent cells. This network consists of three pluripotency genes-the three Yamanaka factors: Oct4, Sox2 and Klf4- and two generic lineage-specific genes (LSGs). The main difference between our model and models previously built is the introduction of epigenetic regulation (ER) of the LSGs, which will enable to account for the effects of metabolism in the reprogramming process[1]. More precisely, ER will be expressed by the acetylation and methylation levels of the LSGs. Acetylation and methylation, as well as deacetylation and demethylation, are assumed to be mediated by some enzymes such as the hystone demethylases (HDMs)[2]. These enzymes are the responsible for the coupling of the differentiation/reprogramming system and the metabolism.

Both asymptotic and numerical methods have been used to study our model for metabolic reprogramming. In the numerical case, Gillespie's stochastic simulation algorithm[3] has been used, whilst for studying the deterministic system, a separation of time-scales together with a quasi-steady state approximation (QSSA) have been applied. We conclude that metabolic transformations normally associated to cancer interfere with the epigenetic regulation of lineage-specific genes, thus enhancing the efficiency of the reprogramming of somatic cells by induction of the Yamanaka factors.

Keywords: reprogramming, cancer, stem cells, oncometabolites, stochastic, Yamanaka factors.
Acknowledgments. N.F-B. and T.A. acknowledge the Spanish Ministry for Science and Innovation for funding under grant MTM2011-29342 and Generalitat de Catalunya for funding under grant 2014SGR1307. T.A. acknowledges support from the Ministry of Economy & Competitivity for funding awarded to the BGSMath under the "María de Maeztu" programme, grant number MDM-2014-0445. This work is supported by a grant of La Caixa Foundation on Collaborative Mathematics awarded to the CRM. This work was supported by grants from the Ministerio de Ciencia e Innovación (Grant SAF2012-38914), Plan Nacional de I+D+I, Spain and the Agència de Gestió d'Ajuts Universitaris i de Recerca (Grant 2014 SGR229), Departament d'Economia i Coneixement, Catalonia, Spain to J.A.M.

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Modelling drug-target binding in a microfluidic 3D cell culture

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Drugs act in the body by binding to receptors which results in an effect. The rates with which the drugs, also called ligand, bind to receptors and with which they detach from the receptors are in general unknown. Moreover, it is very difficult – sometimes even not possible – to measure these binding rates directly in experiments. Our aim is to estimate the binding rates by combining *in vitro* experiments with a mathematical model.

In the experiments, we use a flow channel containing cells with receptors to which the ligand can bind. We produce a flow through this channel of a fluid containing a concentration of ligand. Then, the concentration of the ligand at the end of channel resulting from the input-flow combined with the binding to receptors is measured.

As far as we know, diffusion has so far been incorporated in binding kinetics models (which are ordinary differential equations (ODEs)) by modifying the binding coefficients in the ODE model to take into account the diffusion, as so-called limited diffusion, [1]. We take a new mathematic approach and model this set-up by a system of differential equations for the ligand and the bound ligand-receptor complex. The ligand moves through the channel by advection (flow) and diffusion while simultanuously binding to receptors. The receptors, and hence, also the bound complex is fixed in space. This results in an advection-diffusion equation (a partial differential equation (PDE)) for the ligand coupled to an ordinary differential equation for the bound complex. We study this system of differential equations by numerical simulations and analytical methods.

By combining the results obtained with the mathematical model and the results from the experiments we estimate the order of magnutide of the rates of the binding kinetics.

Keywords: modelling pharmacological processes, system of differential equations.

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Mathematical modelling to understanding the dynamics of signalling pathways initiated by drugs used for the treatment of Asthma.

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We aim to use a mathematical approach that allows understanding signalling pathways initiated by the administration of drugs; used for the treatment of Asthma.

At molecular level, once a drug molecule binds to a receptor on a cell, it activates a cascade of signalling pathways within the cell that lead to the biological effects. Understanding the dynamics of these pathways is a challenging task in drug discovery. We integrate biological knowledge and experimental data to build a set of mathematical models with the aim to investigate the dynamics of these signalling pathways in airway smooth muscle (ASM) relaxation in response to drugs exemplified by Salbutamol and Atropine. We first use ODEs to represent the rates of activation, degradation, and production of the concentration of key signalling molecules, thought to be involved in ASM relaxation. Potential interactions between these molecules are represented by initially unknown parameters. Synthetically generated and experimental data are used to validate the models and identify the unknown parameters. We present results for representative 5-dimension (for Salbutamol) and 10-dimension (for Atropine) models. Our results show that the models perform well with synthetically generated data. With experimental data, the models give expected results when the seven successive experiments were taken as seven samples of a single experiment (enough data for parameters identification).

To get a better insight into the system behaviour, in particular between successive experiments, we build a set of Bayesian networks. The network nodes are the signalling molecules and its edges are the potential interactions between these molecules. Because of the uncertainty over the interactions between the signalling molecules, the inability to measure most molecules concentrations, and the presence of error in experimental data, we assume that the system state propagates between two consecutive measurements according to a probability density, and that the parameters, the initial state of the system, and the concentrations of signalling molecules are random variables. We use the EM algorithm to estimate the state of the system and the parameters that maximise the likelihood of the observation (ASM relaxation). Even though computationally demanding, this approach allows to get a better insight into the dynamics of the system as a whole and, in particular between two successive time experiments.

Our approach can be used to help understand cellular signalling pathways and diseases mechanisms, drug-drug interactions, and hence confirming or denying potential molecular interactions and pharmacological findings.

Keywords: Asthma, Bayesian analysis, EM algorithm, Mathematical modelling, ODEs, Parameters identification, Signalling pathways.
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Solving pharmacokinetic models with the introduction of new mathematical functions

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Combined eliminations have been widely considered in the discovery of new drugs, particularly hormones, to describe their kinetics. Clearance of these drugs generally exhibits parallel elimination mechanisms, involving a linear renal elimination and a nonlinear internalization. The latter is generally represented using a saturable Michaelis-Menten function. The current way to study these drugs is through numerical simulation. However, a mathematical analysis is still lacking. An analytic solution of such models would offer a direct way to thoroughly characterize the kinetics of these drugs. Inspired by the Lambert W function, we introduce a new family of X functions to develop the closed forms of such models. This family generalizes in fact the Lambert W function, and has the latter as an accumulation point. Using X function, we successfully obtained closed forms for single and multiple intravenous bolus administrations for one compartment models. Moreover, we proved that the elimination half-life ($t_{1/2}$) exhibits a dose-dependency and is controlled by the linear elimination pathway. We also clarified the contribution of each elimination pathway and delineated dominant kinetics in terms of model parameters and the different levels of drug concentration. Finally, we mathematically proved the convergence of multi-dose kinetics towards a stable kinetic status.

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MS16: Recent developments and applications of isogeometric methods

MS16: Recent developments and applications of isogeometric methods

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Isogeometric Analysis (IGA) refers to a collection of methods that use B-splines, or some of their extensions such as NURBS, T-splines or hierarchical splines, to approximate the solution of problems governed by partial differential equations (PDEs). The method was introduced by T.J.R. Hughes and coworkers in 2005, with the aim of improving the interaction between CAD and CAE software, by using the same kind of functions both for the geometric representation of the design and for the solution of the PDEs.

More than ten years after the publication of the first seminal paper, the development of a true CAD/CAE interaction based on IGA remains an open problem. However, one of the most interesting features of isogeometric methods is the high smoothness of splines with respect to standard classical finite elements, which has already shown its benefits in several situations. For instance, splines of high regularity allow to introduce new discretization schemes for high order PDEs, they improve the accuracy in terms of degrees of freedom, and also allow an easier geometry manipulation and deformation during the simulation process.

Although computational solid mechanics is the main field of application of IGA, the potential advantages of the method with respect to standard finite elements have attracted the attention of researchers from different areas, and IGA has been already applied in many other fields, such as fluid mechanics, fluid-structure interaction and electromagnetism, for instance.

This versatility of IGA is also reflected by the presentations of this minisymposium, with two works on computational solid mechanics, one in computational electromagnetism and one in computational fluid mechanics. The work by P. Antolin is devoted to the development of a new solid shell formulation that avoids locking and is computationally efficient. The one by H. Casquero, also related to computational solid mechanics, applies IGA collocation methods with local refinement by T-splines to high order shell models, and with the interesting feature of a direct CAD/CAE interaction. The paper by J. Corno presents the study of IGA in combination with domain decomposition methods, with particular interest in electromagnetism and in the simulation of cavity accelerators. Finally, the work by C. de Falco is devoted to the simulation of blood circulation in the human liver, considering the Darcy-Stokes-Brinkmann equation to model multiscale phenomena, and which is numerically solved using div-conforming spline spaces.

Hugo Casquero. Universidade da Coruña (Spain). *Analysis-suitable T-splines of arbitrary degree: From isogeometric collocation to fully nonlinear Kirchhoff-Love shells.*

Pablo Antolin. Università degli Studi di Pavia (Italy). *An isogeometric solid shell element for large strain problems.*

Jacopo Corno. TU Darmstadt (Germany) and Politecnico di Milano (Italy). *IsoGeometric State Concatenation Method for Reduced Order Simulation of Complex Accelerator Cavities.*

Carlo de Falco. Politecnico di Milano (Italy). *Isogeometric Simulation of the Perfusion Characteristic of Liver Tissue.*

Analysis-suitable T-splines of arbitrary degree: From isogeometric collocation to fully nonlinear Kirchhoff-Love shells

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T-splines were introduced in both design and analysis in order to overcome the main limitations that NURBS have in those two fields. Analysis suitable T-splines (ASTS) of arbitrary degree are a noteworthy subset defined in [1]. This subset of T-splines enables to perform local h-refinement on two-dimensional and surface meshes while maintaining all the important mathematical and geometrical properties that NURBS possess such as, e.g., polynomial partition of unity, linear independence, optimal convergence rates, nested spaces, pointwise non-negativity of the basis functions, among others.

In [2], we present isogeometric collocation methods for second- and fourth-order problems using the aforementioned T-spline subset. The proposed methods are highly efficient as the approximation order increases since only one point evaluation is needed per degree of freedom. Moreover, highly nonuniform meshes without high aspect ratios can be constructed, this allows us to collocate Neumann boundary conditions in a straightforward manner without the appearance of numerical instabilities. In [3], we aim at bringing closer a seamless and flexible integration of design and analysis for thin shells through the use of ASTS, which includes the reparameterization of trimmed NURBS surfaces coming from the industrial CAD program called Rhino.

In both applications, the local h-refinement capabilities of ASTS of arbitrary degree enable them to signficantly outperform their NURBS counterparts.

Keywords: Isogeometric analysis, Analysis-suitable T-splines, Arbitrary-degree T-splines, Collocation, Nonlinear Kirchhoff-Love shells, Trimmed surfaces

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An isogeometric solid shell element for large strain problems

Pablo Antolin[1], **Annalisa Buffa**[2], **Josef Kiendl**[3], **Marco Pingaro**[1], **Alessandro Reali**[1,2], **Giancarlo Sangalli**[1,2]

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The simulation of thin structures like shells is an important class of problems which can be effectively tackled by means of Isogeometric Analysis (IGA). In this work, we focus on the family of shell formulations referred to as "solid shells", where the simulation of shell-type structures is performed by means of a mesh of 3D solid elements, with typically only one element through the thickness. Solid shells are particular attractive because, on the contrary of bivariate shells, they allow simple treatment of double-sided contact situations and coupling with 3D solid elements. In addition, standard 3D constitutive models can be readily used without the need of model reduction procedures or special interfaces. However, we have to highlight that using a single element through the thickness calls for special treatments to alleviate the unavoidable presence of (shear, curvature thickness, and membrane) locking phenomena. Taking inspiration from standard finite elements, several cures for locking have been already proposed in the literature and others may be considered, ranging from $\bar{B}$ to enhanced strains. An interesting and inexpensive approach in this sense could be found within the family of Assumed Natural Strains (ANS), which have already been proven to be effective within the IGA framework.

Within this context, we herein present a novel ANS solid shell formulation for the analysis of large strain problems. The formulation is fully consistent and general, and allows to obtain results comparable to those attained by cubic elements (practically locking-free but expensive) using a much cheaper quadratic approximation. Extensive numerical testing proves the good behavior of the proposed formulation in different demanding situations.

IsoGeometric state concatenation method for reduced order simulation of complex accelerator cavities

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In the numerical modelling of linear accelerator structures, the simulation domain is often restricted to single RF cavities, since the direct numerical treatment of the whole chain is too computationally expensive. The resource requirements in terms of both CPU time and memory become even more challenging when a large number of simulations needs to be performed, as is the case for, e.g., uncertainty quantification or shape optimization.

The use of IGA in cavity simulation has been proven to be beneficial both in terms of accuracy and of overall reduction of the computational cost [1, 2]. However, the simulation of large and complex structures remains an overwhelming task.

In order to overcome these difficulties we consider the extension to the IGA setting of the State Space Concatenation (SSC) method recently introduced by Flisgen et al. [3, 4]. In the SSC approach, the complete computational domain geometry is decomposed into smaller sub-domains in which the fields are modelled by means of low dimensional modal bases. By placing the interfaces between neighbouring sub-domains at suitable locations, where the domain geometry approaches that of a waveguide, physical knowledge about the waveguide dispersion relation may be exploited to a priori select the most relevant elements of the local modal bases. The model for the complete system is then recovered by treating each sub-domain as a dynamical system with given Input/Output characteristics and by coupling the I/O "ports" of neighbouring cells.

In order to study the accuracy and stability properties of the IGA/SSC method, we cast it into the form of standard Domain Decomposition methods. As a by-product, our more abstract representation of the SSC allows for straightforward extension of the approach to other physical applications ranging from Quantum Mechanics to Structural Vibrations.

Keywords: Domain Decomposition, Isogeometric Analysis, Linear Accelerator, State Space Concatenation.
Acknowledgements: This work is supported by the 'Excellence Initiative' of the German Federal and State Governments and the Graduate School of Computational Engineering at Technische Universität Darmstadt.

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Isogeometric simulation of the perfusion characteristic of liver tissue

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In the last decades, the biomedical relevance of mathematical models has been demonstrated and comparison of experiments against computer simulations has been encouraged. Blood circulation in the human liver and in particular perfusion, the process of delivering blood to the capillary bed, is an open problem and inherently multiscale in nature. Models currently available in the literature [2, 1] either present a macroscale approach in which liver is assumed as a homogeneous anisotropic porous medium and therefore flow within it is simulated using Darcy's equation, or they work at the microscale where the vascular and extravascular domains need to be treated differently solving Stokes' equation in the former and Darcy's equation in the latter and applying suitable coupling condition at the interface. In this communication, instead, we present an approach where the Darcy-Stokes-Brinkmann [3] equation is used on the entire computational domain, different areas of the tissue being represented by a (possibly discontinuous) friction coefficient. This approach allows to run simulations at the capillary scale on real-life geometries deduced from medical images avoiding complex and costly preprocessing such as edge detection, and mesh generation. The peculiar properties of IsoGeometric discretization methods [4, 5] such as stability and ability to provide exactly divergence free velocity are exploited in the simulation. After validating the numerical method on 2D and 3D test cases based on syntetic images, we apply it to actual micro-CT images of the liver and perform an upscaling procedure to determine the macroscale parameters of the tissue such as the local permeability tensor.

Keywords: multiscale modeling, incompressibility, isogeometric analysis, stokes flow, porous media.
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MS17: MODCLIM - Erasmus+ project

MS17: Minisymposium title: MODCLIM – Erasmus+ project

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MODCLIM is an integrated research training course and problem solving workshop for challenging mathematical and computational problems from industry and applied sciences. During each of the years of the project, a group of 20-30 PhD and advanced undergraduate (MSc) level students are trained, and 4-6 industrial problems from leading edge technological development are worked through. The project unites a number of ECMI partners (all of whom have experience in running a Masters programme in industrial mathematics and have contacts with industry in their region) but is also the first one of this kind in the Sub-Mediterranean area and an important step towards cross-mediterranean collaboration in industrial mathematics.

The purpose is to train MS students and PhD students in research skills of applied mathematics. The project concentrates on practical problems coming from real world and results in development of research capacity in applied mathematics, spur science and technology education. Moreover, MODCLIM prepares the students (many of whom being future academicians) in a mild way for Study Groups. The difference is that with MODCLIM the students get a proper introductory course and training tasks related to the real life modeling problem, whereas during a Study Group participants would have to search and understand the same concepts in just under a week.

The partners involved in MODCLIM are all ECMI nodes. The project was created in the spirit of ECMI's Modeling Weeks and Study Groups. The idea was to expose the students to real industrial problems, including the training school necessary for them to grasp the problem the students would work on.

Speakers:

Juan Rocha. University of Las Palmas Gran Canaria (Spain). *Modeling Clinic for Industrial Mathematics: A collaborative project under Erasmus+ program.*

Matylda Jabłońska-Sabuka. Lappeenranta University of Technology (Finland). *The importance of synergies among mathematical modeling activities: MODCLIM - ESGI example.*

Florian Gensheimer. Mathematical Institute, University of Koblenz-Landau (Germany). *MODCLIM 2015: A student's point of view.*

Thomas Götz. University of Koblenz, Landau (Germany). *MODCLIM 2016 - Review of the Modeling Clinic at Koblenz University".*

Giovanni Russo. Department of Mathematics and Computer Science, University of Catania (Italy). *MODCLIM Training school, Catania 14-27 February 2016.*

Keywords: mathematical modeling, modeling clinic.

Modeling clinic for industrial mathematics: A collaborative project under Erasmus+ program

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The *Strategic Partnership for the Development of Training Workshops and Modeling Clinic for Industrial Mathematics* (acronym MODCLIM) is a strategic partnership for higher education project, approved in 2014 by Erasmus+ program, Key Action 2: Cooperation for innovation and the exchange of good practices.

MODCLIM develops a project focused on mathematical technologies needed for the progress of industry and novel engineering solutions. The project pretends to contribute in addressing the challenges that industrial mathematics, as part of the next generation of methodologies in research and development and knowledge management, represents for university education, curriculum development, training practices and research collaboration. With this aim, MODCLIM project has developed two cycles, along the years 2015 and 2016, for training two groups of 20-25 PhD and advanced undergraduate level students (MSc, BSc), addressing different industrial problems from leading edge technological development. Each cycle has three interconnected steps: Training School, Intermediate online-project and Modeling Clinic; and a Final Project Report.

The project concept is a novel approach that assimilates features from prior European experience (see [1] and [2]) and successful innovative models overseas, like RIPS's model from USA (see [3]). Further information about MODCLIM project is available through the website http://modclim.ulpgc.es.

Keywords: Industrial mathematics, industrial applications, modeling and simulation, mathematical technologies, modeling of industrial processes.
Acknowledgments. We would like to acknowledge the support of the Erasmus+ Program for funding the MODCLIM project; as well as the support of all the universities and entities involved in MODCLIM project, and the collaboration of the teachers and students who have participated throughout the project.

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The importance of synergies among mathematical modeling activities: MODCLIM – ESGI example.

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On September 7-11, 2015 a one-week problem solving workshop took place in Lappeenranta, Finland in conjunction with ESGI 112 workshop. The topic of the event was mathematical and computational projects coming from industry. This Modeling Clinic was carried out using the Mathematical Study Group format (http://miis.maths.ox.ac.uk/). The audience was introduced to seven problems coming from the field of industrial mathematics. Four of the problems were coming from or inspired by the MODCLIM Training school items (an event which took place half a year before the workshop in Lappeenranta). Additional 3 problems came from industrial companies in Finland and Russia.

The workshop ESGI 112/MODCLIM brought together an audience from various origins and about 13 countries. The participants were mathematicians and doctoral students of applied mathematics and engineering who are interested in research questions coming from applications in industry and applied sciences. In total, about 40 academic guests, professors and doctoral students, coming from 9 European countries and from universities in Russia, Balkans, Tanzania, India and Algeria.

ESGI workshops of industrial mathematics have been organized in various parts of the world for many years. LUT has organized in the past three similar workshops in collaboration with St Petersburg State Polytechnic University. This time the event was bigger because of the additional partners from the Erasmus+ project MODCLIM. Moreover, a study group would usually bring together academicians from doctoral student onwards, with majority of post-docs and professors, whereas in our event there were as many junior participants (starting from MSc level) as the senior ones, but at the same time facing problems much more difficult and real-life oriented than a similar student-oriented event, the so-called Modeling Week.

This talk will present the benefits of having merged these events for both the organizers and participants.

Keywords: mathematical modeling clinic, modeling workshop, study group, project synergy
Acknowledgments. Partially supported by the Erasmus+ Strategic Partnership project MODCLIM.

MODCLIM 2015: A student's point of view

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In this talk, I want to reflect my experiences as a participating PhD student of the last year's MODCLIM (Modeling Clinic for Industrial Mathematics) event in Las Palmas and Lappeenranta. MODCLIM is a project of several European universities that is intended for PhD and advanced undergraduate (MSc, BSc) level students. It consists of a training course and a problem solving workshop. The project aims at bringing together mathematical knowledge from different areas and learning how industrial problems can be modeled and solved mathematically. In my talk, I will describe the organization and the different phases of the project from my view as a participant. Furthermore, I want to inform about the mathematical topics and industrial problems that occurred in the last year's project. Finally, I will talk about the advantages of participating in the MODCLIM project for a student.

Keywords: MODCLIM

MODCLIM 2016 — Review of the modeling clinic at Koblenz University

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The Erasmus+ project "Strategic Partnership for the Development of Training Workshops and Modeling Clinic for Industrial Mathematics" (MODCLIM, http://modclim.ulpgc.es) is about an integrated research training course and problem solving workshop for challenging mathematical and computational problems from industry and applied sciences.

In it second year, Masters and PhD–students from several European Universities participated in a two–week training school in February in Catania, Italy. During this training school, courses on subjects like Principal Component Analysis, Image Analysis, Smoothed Particle Hydrodynamics and Dynamic Network Optimization were given. The second phase consisted of the one–week Modeling Clinic held in May at the University in Koblenz, Germany. In this talk we will report on the outcome of the second year of MODCLIM and discuss ideas for a continuation of the project.

MODCLIM Training School, Catania 14-27 February 2016

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MODCLIM Training School, Catania 14-27 February 2016.

The aim of this short talk is to give an overview of the MODCLIM training school held in Catania last winter. This in order to share our experience, the difficulties we encountered, and the solutions we found in managing the event.

The school was the third event of the series, the preceding ones being held in Las Palmas, Spain (March 2015), Lappeenranta, Finland (September 2015). The last event of the series is the problem solving workshop that takes place in Koblenz, Germany, in May 2016. For more details, please take a look at the MODCLIM web page, http://modclim.ulpgc.es.

In the two weeks of the Catania Training School, the following courses were offered:

Week 1: February 15-19, 2016
- *Extracting information from data: Principal Component Analysis, Robustness, and Outlier Detection*, **M. Rosário Oliveira**, Lisbon.
- *Image Analysis. Focus on image restoration based on variational models*, **Susana Serna**, Barcelona

Week 2: February 22-26, 2016
- *Smoothed particle hydrodynamics for non Newtonian fluids and applications*, **Giuseppe Bilotta**, Catania.
- *Dynamic Network Optimization and Applications in Civil Security*, **Jan Ohst**, Koblenz

The school was attended by 15 students, regularly enrolled in the program: four from Italy, three from Spain, two from Finland, two from Portugal, two from Germany and two from Poland. In addition, four undergraduate students from the University of Catania asked to attend the class, given the great interest of the topics. Given the relatively low cost of the local students, the enlargement of their number could be a way to increase the impact of the school for a given budget.

In addition to the training courses, two visits of local research laboratories were organized. The first one was the visit to the IPLAB (Image Processing Laboratory), a lab within the Department of Mathematics and Computer Science, (http://iplab.dmi.unict.it), devoted to the development of image processing techniques, and their application to art restoration, pattern recognition, forensics, and so on. Dr. Giovanni Maria Farinella guided the students, giving a brief overview of the various activities of the lab.

The second visit took place at the Catania section of INGV, the National Institute of Geophysics and Volcanology (http://www.ct.ingv.it/it/). The event, jointly organized by Dr. Ciro Del Negro and G.R., took the whole morning of Friday February 26th, and consisted of a guided visit of the modeling group to the INGV, followed by a cycle of seminars on "Uncertainty Quantification in Lava Flow Hazard Monitoring".

Local expenses were administrated by DMI, with the MODCLIM funds. A very careful management of the expenses allowed to support all the students lodging and living expenses.

Keywords: Training Courses, Industrial Mathematics, Principal Component Analysis, Image Restoration, Non Newtonian Fluids, Dynamic Network Optimization
Acknowledgments. Partially supported by the European Erasmus+ project MODCLIM, Modeling Clinic for Industrial Mathematics (http://modclim.ulpgc.es).

MS18: 8 years of east African technomathematics

MS18: 8 years of East African Technomathematics

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Lappeenranta University of Technology, with the help of funding from the Finnish Ministry of Foreign Affairs, has now for eight consecutive years supported the development of applied and industrial mathematics in the East African region. The collaboration started from North-South-South exchange projects where students from the South would get the chance to visit LUT for study periods from 5 to 9 months. Over the last three years our activities have also extended into revision of the Applied Mathematics curricula in the East African universities, as well as establishment of contact between local industries and academia to enhance research collaboration and applicability.

This minisymposium will give an overview of the collaboration, the success stories and challenges we have faced on the way. This will include:

- the history of how the collaboration was initialized and carried on,
- the inspirations gained from the activities organized in partner African countries (like the training of instructors for Modeling Weeks),
- promotion of mathematical sciences in East African region, i.e. through AIMS Tanzania,
- personal student/teacher point of view on the collaboration,
- and tangible capacity building outputs, like creation of new study programmes.

Speakers:

Matti Heiliö, Lappeenranta University of Technology (Finland). *Building Applied Mathematics Knowledge Base in East Africa.*

Tuomo Kauranne, Lappeenranta University of Technology (Finland). *Win-Win-Win projects: How to run African and European industrial collaboration projects in Technomathematics.*

Godwin Kakuba, Makerere University (Uganda). *Modelling weeks: the European and Tanzanian experience from a student's/instructor's point of view.*

Matylda Jabłońska-Sabuka, Lappeenranta University of Technology (Finland). *The training of instructors for Mathematical Modeling Weeks – a new concept born from LUT-East Africa collaboration.*

Wilson Mahera Charles, African Institute of Mathematical Sciences (Tanzania). *AIMS - Promoting the Mathematical Sciences and their Applications.*

Keywords: technomathematics, AIMS, capacity building, mathematical modeling in developing counties.

Building applied mathematics knowledge base in East Africa

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Lappeenranta University of Technology has coordinated two projects involving 8 universities in East African region: (1) East Africa Technomathematics 2007-2015 and (2) Mathematics education and working life relevance 2013-2015. The aim is to transfer to African colleagues the ideas and encouragement that ECMI stands for, to promote awareness about real world impact of mathematics. The projects are funded by the Finnish Ministry of Foreign Affairs and administered by The Finnish Center for International Mobility CIMO. The objective is to open up opportuni-ties for cooperation between higher education institutions in Finland and developing countries. The focus is capacity building and student and teacher exchange.

A weakness in mathematics education in third world countries is often the missing touch with applications. The educational culture fails to bring forward how to apply mathematics to the benefit to society. The aim of our project is to enrich the higher education culture by illuminating the real world context, the possibilities of interaction with stakeholders in society. The activities are meant also to facilitate "within East-Africa" network effects and encourage female students to seek careers in technology and science.

The project plan has included student exchange on MS/PhD studies level, staff visits, intensive courses including three Modelling Weeks, workshops on curriculum questions, university-industry interaction, challenges on teacher training. Partners are universities in Tanzania, Rwanda, Uganda, Kenya and Ethiopia and 3 universities from Finland.

The project has helped to increase MSc production locally. Also a number of MSc degrees and PhD degrees have been generated as an output from the exchange. We have promoted curriculum modifications, MatLab skills, data assimilation methods, weather models, applied statistics, statistical analysis of model reliability by MCMC methods. An important feature has been introduction of Modelling Week concept, a novel idea in the region. Several students who have graduated as the result of the cooperation are now employed as staff members of their department, or gained professional positions in financial or governmental institutions. The latter also proves that the society is ready to think of mathematics graduates not only as future math teachers, but also skilled professionals in various areas.

There is obvious demand to broaden the cooperation between Africa and the European applied mathematics community. The skills and knowledge reservoir that ECMI contains could have a big influence in the development of technology, applied sciences and public governance. Objectives would be increased skills in modelling, ICT tools and quantitative methods in engineering, agriculture, environmental issues, energy sector to name a few. To influence the skills and aptitude of the next generation of mathematics teachers is another big task.

Keywords: Africa, technomathematics, modelling, working life
Acknowledgments. The work is supported by The Finnish Center for International Mobility CIMO.

Win-Win-Win projects: How to run African and European industrial collaboration projects in Technomathematics

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Mathematics transcends countries, continents, cultures and languages. It therefore provides a rare opportunity for truly interational collaboration. But if we wish mathematics to have a lasting impact, we need to make it relevant to the societies to which it is introduced.

European, African, American and Asian social contexts differ widely from each other. Therefore the applications of mathematics must also differ, if mathematics is to have an impact in each of these continents. In this talk I shall go through many examples of inter-continental industry-society-academia projects that each illustrate one or more aspects of these differences. Examples will cover both successes and failures. Hopefully they will also provide guidance for other universities embarking upon trans-continental efforts on how to navigate in the rich but challenging global reality that we inhabit.

Modelling weeks: the European and Tanzanian experience from a student/instructor's point of view.

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Europe probably has a long history of mathematical modelling and the idea of modelling weeks is certainly much more rooted in Europe than it is in East Africa. In fact, it could be a new idea in East Africa, thanks to CIMO. During my PhD studies at Technische Universiteit Eindhoven, the department once hosted the modelling week in 2008. Then I had a chance to take part in some group work but as a student. I have also had the opportunity to take part in one of the modelling weeks at the University of Dar-es-Salaam, the third East Africa technomathematics modelling week that took place from 11th - 15th August 2014, but as an instructor. It is this experience of both student and instructor that I share in this presentation.

Although the students are to solve the problems presented in form of small projects in modelling weeks, as an instructor the challenge is not only to pose the problem but also to guide the students or participants to the solutions.

Modelling weeks are problem solving workshops whether in Europe or in East Africa. The scale of industrialisation in these two regions will drive the intensity and kind of projects that are tackled at these workshops. The projects discussed are meant to be based on real life problems, and "real life" may vary from place to place. This may initially prove to be a challenge for East African countries like Tanzania.

The other interesting trait at these modelling weeks is the partnership between industry and academia. This bond is vital for the success of these modelling weeks since, although the activity is academic in nature, the industry will be instrumental in providing both the real life problems and the financing. The initiators of the idea in Tanzania may need to add another dimension to the project, something that will make sure that eventually it is a consortium of east African or African for that matter, institutions and industries that are spearheading the modelling weeks.

However, the timing for such a project in East Africa could not have been better as the region struggles to adapt to local research driven industrialisation. There is no doubt that this is an initiative that will go a long way in catalysing the development of science and technology in East Africa.

Keywords: Modelling, modelling week, industrialisation
Acknowledgments. Thanks to HEI-ICI programme of CIMO that facilitated my participation to the modelling week in Tanzania and this presentation.

The training of instructors for Mathematical Modeling Weeks – a new concept born from LUT-East Africa collaboration.

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Lappeenranta University of Technology has coordinated a project involving 8 universities in Tanzania, Rwanda, Uganda, Ethiopia and Kenya, namely East Africa Technomathematics 2007-2015. The aim was to transfer to African colleagues the ideas and encouragement that ECMI stands for, to promote awareness about real world impact of mathematics. The project was funded by the Finnish Ministry of Foreign Affairs and administered by The Finnish Center for International Mobility CIMO. The knowledge exchange was carried out mainly through exchange mobility periods of students and stuff, as well as intensive courses.

On European ground, one of the most powerful tools for spreading the concept of industrial mathematics among students and academicians are study groups and modeling weeks. Therefore, within our initiative in the developing countries we have decided to incept also the modeling week idea onto the African environment.

The history of European modeling weeks dates back to 1980s, but since this idea was new to most of our colleagues in East Africa, we decided to extend the classical event by preceding it with a training of instructors. The idea was to familiarize the group instructors with the pedagogical aspects of the modeling week. The following points have been discussed with the future supervisors

- the history of the ECMI modeling weeks,
- what is a good problem for a modeling week,
- the benefits from participation for both students and instructors,
- how to lead and mentor the students through the course of the week, keeping in mind that it should be the students who do the actual modeling and solution, and not the instructor,
- how to break down the problem into subproblems to help the group manage resources and time.

As a result, each of the modeling problems brought by our East African colleagues to the event were pre-discussed so that the instructors would know how to lead the groups. Moreover, each of the new instructors was paired with another colleague who already had such an experience from ECMI modeling weeks (whether as a student or an instructor).

In the course of the project we have realized that such a training would be much in place also during the ECMI events, where ofter inexperienced doctoral students take the challenge of being group instructors. As it has been noticed from numerous discussions and interviews with them, if they have not attended the event themselves, neither as a student nor as an instructor before, they rarely know the right way to mentor and ”tease” the group towards finding the solution.

Keywords: modeling week, training of instructors, problem breakdown
Acknowledgments. The work was supported by The Finnish Center for International Mobility CIMO.

AIMS - Promoting the mathematical sciences and their applications

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African Institute for Mathematical Sciences, Tanzania The African Institute for Mathematical Sciences is a Pan-African network of Centres of Excellence for Postgraduate Training, Research and Public Engagement in the Mathematical Sciences. The Centres are centrally coordinated by the AIMS Next Einstein Initiative's Secretariat which is now headquartered in Kigali, Rwanda. Their target is to establish 15 such Centres across Africa by 2023. AIMS Tanzania is the fifth and latest to one and has now been operational for almost two years. The next Centre will be AIMS-Rwanda opening in August 2016. The scope of these Centres is captured by: "From health research to information and communications technology, from finance and banking to climate forecasting, mathematical skills are the backbone of modern societies. Research shows that investment in university-level education in Africa may well be the fastest route to technological catch-up and economic development." AIMS Tanzania has benefited in many ways from cooperation with Europe, including with ECMI nodes such as Lappeenranta University of Technology. Research visits, staff exchanges, workshops and courses have been organised with AIMS Tanzania's close partner, the University of Dar es Salaam, for the past 9 years and now cooperation with AIMS itself is developing. AIMS Tanzania is ideally situated and resourced and has considerable potential as a hub connecting African colleagues interested in industrial mathematics to ECMI nodes interested in Africa. The talk will focus on AIMS history from 2003 to 2016, its postgraduate training model, including its structured curriculum, student recruitment, course delivery and assessment. It will also describe the AIMS Industry Initiative and touch on the three other pillars of AIMS namely Research, Teacher Training and Public Engagement. Examples of current research and student projects inspired by 'real world' problems will be described. The conclusion will summarise the successes and challenges of AIMS.

Keywords: AIMS

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http://www.nexteinstein.org/

MS19: Theoretical and practical aspects of photoacoustic imaging

MS19: Theoretical and practical aspects of photoacoustic imaging

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This minisymposium consists of 5 talks that concentrate on theoretical and practical aspects of photoacoustic and thermoacoustic tomography (in short PAT and TAT). PAT and TAT are very promissing hybrid methods, more precisely, the tissue is exposed to laser light (first mode) that causes a pressure wave propagating to the boundary of the tissue and the pressure at the boundary (second mode) is measured. The goal is to estimate the electromagnetic absorption of the tissue with the help of these pressure data. Due to the nature of PAT and TAT, tumors and cyst produce a high contrast in their images, but these methods are limited to "transparent tissue" like the human breast. This minisymposium focuses on reconstruction formulas for PAT with and without dissipation, PAT for dissipative media in which one or several relaxation processes take place, PAT for stratified media and Interferometric wave source inversion in PAT.

Speakers:

Laurent Seppecher. Massachusetts Institute of Technology, Cambridge (United Kingdom). *Interferometric wave source inversion for photoacoustic imaging.*

Richard Kowar. University of Innsbruck (Austria). *Theoretical and numerical investigation of time reversal in photoacoustic imaging for dissipative media with time relaxations.*

Cong Shi. University of Vienna (Austria). *A reconstruction method in photoacoustic tomography in weak attenuation case.*

Margaux Vauthrin. Laboratoire Jean Kuntzmann, Grenoble (France). *Photoacoustic imaging in stratified media.*

Keywords: photoacoustic imaging, thermoacoustic imaging, time reversal, source inversion, backprojection formula.

Interferometric wave source inversion for photoacoustic imaging

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Inherent issues with practical wave source inversion for photoacoustic imaging bring instability and defocusing in the reconstructed image. This is caused by natural uncertainties on background wave speed, biological displacements of the tissue, electronic noise, etc...

I propose in this talk a new way of inverting the wave source problem from interferometric data. I will describe the theoretical and practical aspect of this inversion and explain the expected gain of stability to these natural uncertainties. In particular, we will discuss the natural auto-focusing behavior of this technique. Of course, this idea may be relevant in many other inverse problems involving oscillating forward operators with uncertainties.

Our interferometric approach to solve the linear problem

$$Fs = d$$

consists in minimizing the quartic cost function

$$J_E(s) = \sum_{i,j} E_{i,j} \left((Fs)_i \overline{(Fs)_j} - d_i \overline{d_j} \right)^2$$

where E is a sparse symmetric boolean matrix. The choice of this sparse filter E plays an essential role on the stability of the method. I will propose a general strategy to choose this matrix depending on the type of expected errors and the geometrical setting. I will also discuss the technique used to minimize the non convex cost function J_E.

Keywords: Helmholtz equation, inverse source problem, interferometric imaging, correlation fitting, quartic optimization.

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Theoretical and numerical investigation of time reversal in photoacoustic imaging for dissipative media with time relaxations

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This talk is concerned with theoretical and numerical investigation of time reversal in photoacoustic and thermoacoustic tomography (PAT and TAT) of dissipative media that are similar to water and which undergo one or several time relaxation processes. We present a generalization of the wave equation of Kowar, Scherzer and Bonnefond which models several relaxation processes and compare it to the wave equation of Nachman, Smith and Waag. In particular, we discuss their "time reversal properties". Moreover, we discuss the numerical implementation of the wave equation of Nachman, Smith and Waag and present some numerical examples.

Keywords: Photoacoustic imaging, dissipative wave, wave equation of Nachman Smith and Waag.

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A reconstruction method in photoacoustic tomography in weak attenuation case

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In this talk I will present our new reconstruction method for photoacoustic imaging in the weak attenuation case. It is an explicate reconstruction formula and it works for spherical observation surface. First I will introduce the classical no attenuation reconstruction methods, then introduce how we get this formula and the difference between them. In the second part, I will give some numerical results, including 1D and 3D.

Photoacoustic imaging in a piecewise constant medium.

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Photoacoustic imaging is based on the photoacoustic effect: an acoustic wave is generated by the absorption of optical energy and it is measured with transducers distributed on the boundary of the object. This imaging technique combines the ultrasonic resolution and the high contrast due to optical absorption. The photoacoustic effect in a bounded domain Ω is described mathematically by the following equations:

$$\begin{cases} -\nabla \cdot D(x)\nabla u(x) + \mu_a(x)u(x) = 0, & x \in \Omega \\ u(x) = g(x) & x \in \partial\Omega \\ \dfrac{\partial^2 p(x,t)}{\partial t^2} - c(x)^2 \Delta p(x,t) = 0, (x,t) \in \Omega \times [0,T] \\ p(x,0) = \Gamma(x)\mu_a(x)u(x) = F(x), & x \in \Omega \\ \dfrac{\partial p(x,0)}{\partial t} = 0, & x \in \Omega \end{cases}$$

The photoacoustic inverse problem has two steps, the first one is the inversion of the diffusion equation and the second one is the inversion of the acoustic equation. This work is about the acoustic inverse problem only. From the acoustic measurements on the boundary we reconstruct the initial pressure $F(x)$ in Ω.

The acoustic speed is often considered as a constant equal to the acoustic speed in water, but the variations in biological tissues can be of 10%. The aim of this work is to find a model for the acoustic speed in order to improve the reconstruction of the initial pressure. We present a method for acoustic speed correction in a biological medium. We consider that in the case where the object contains only water and blood, the acoustic speed depends on the absorption coefficient μ_a.

In the case of a piecewise constant medium, the initial pressure and the acoustic speed will then present the same singularities. This acoustic speed model is then used to perform the inversion of the acoustic equation and to improve the reconstruction of the initial pressure. We use both time reversal and minimization method to perform the reconstruction.

Keywords. photoacoustic, acoustic speed, piecewise constant.
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MS20: Computational electromagnetism

MS20: Computational electromagnetism

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Electromagnetic phenomena is one of the fundations of modern technology and developing models, approximation methods and software tools for electromagnetics computations have a direct impact and great relevance in industry. In the past thirty years computational electromagnetism has became also a prolific and strengthened research field on applied mathematics. The aim of this minysimposium is to bring together a small group of engineers and mathematicians working on common interests to present advanced topics on modeling and discretization of electromagnetic fields and to discuss the effective impact on industrial applications and software design of these advanced techniques.

Speakers:

Stefan Kurz. Graduate School of Excellence Computational Engineering, Darmstadt (Germany), and Tampere University of Technology, DEE-Electromagnetics, Tampere (Finland). *Structure Preserving Mesh Coupling for Maxwell's Equations*.

Holger Heumann. INRIA, EPI CASTOR, Sophia Antipolis (France). *Overlapping mortar methods for axisymmetric plasma equilibria in tokamaks*.

Andrei Kolyshkin. Riga Technical University, Riga (Latvia). *Eddy current testing models for the analysis of corrosion effects in metal plates*.

Pilar Salgado. Department of Applied Mathematics, Universidade de Santiago de Compostela (Spain). *Numerical simulation and optimization of induction heating in forge applications*.

Maryam Khaksar Ghalati. CMUC, Department of Mathematics, University of Coimbra (Portugal). *Stability and convergence of fully explicit leap-frog DG scheme for solving 2D Maxwell's equations in anisotropic materials*.

David González-Peñas. Departamento de Matemática Aplicada e Instituto Tecnológico de Matemática Industrial (ITMATI). Universidade de Santiago de Compostela (Spain). *Thermo-electromagneto-hydrodynamic numerical simulation of the removal of volatile impurities in molten metals*.

Alain Bossavit. GeePs (ex. LGEP), Centrale-Supelec, Gif-sur-Yvette (France). *Topics in Magnetic Force Theory: Some avatars of the Helmholtz formula*.

Keywords: Computational electromagnetics, mathematical modelling, electrostatics, magnetostatics, wave propagation, induction heating, metallurgy, forge applications, ferrofluids, plasma equilibria, tokamaks, optimization, eddy currents, numerical simulation, computational cohomology, discontinuous Galerkin method, nonconforming interfaces, mortar methods.

Structure preserving mesh coupling for Maxwell's equations

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The state of the art for mesh coupling at nonconforming interfaces is presented and reviewed. Mesh coupling is frequently applied to dealing with motion in electromagnetic actuators [1, 2, 3]. The focus of the contribution is on lowest order Whitney elements. Both interpolation- and projection-based methods are considered [4]. In addition to accuracy and efficiency, we emphasize the question whether the schemes preserve the structure of de Rham complex, which underlies Maxwell's equations.

Projection methods require the inversion of a mass matrix. This can be done efficiently by using biorthogonal bases for the Lagrange multiplier space [3, 5], resulting in a diagonal mass matrix. Nevertheless, projection methods are demanding to implement since discontinuous functions have to be numerically integrated. Strategies to cope with this are presented in [6, Fig. 9], [7] and [8, Sect. 3].

The generalization of projection based methods from nodal to edge elements is not obvious. In particular, only a few references aim at a rigorous theoretical analysis of such mortar element methods [9, 10]. Many authors again use the edge element space as the Lagrange multiplier space, e.g. [2, 6, 11]. Unfortunately, this policy does not yield a structure preserving discretization. As a new contribution, a projection method is presented, in which mortar spaces are chosen from the Buffa-Christiansen complex [12]. This approach is structure preserving. Its performance is compared with a straightforward interpolation based on Whitney and de Rham maps.

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Disclaimer: This paper is based on [13]. Similar work was presented at the 16th IEEE Conference on Electromagnetic Field Computation CEFC 2014, and at the 12th Söllerhaus Workshop Fast BEM in Industrial Applications 2014.

Overlapping mortar methods for axisymmetric plasma equilibria in tokamaks

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Existing finite element implementations for the computation of free-boundary axisymmetric plasma equilibria approximate the unknown poloidal flux function by standard continuous finite elements with discontinuous gradients [1]. The location of critical points of the poloidal flux, that are of paramount importance in tokamak engineering, is constrained to nodes of the mesh, which leads to undesired jumps in transient problems. Moreover, recent numerical results for the self-consistent coupling of equilibrium and resistive diffusion suggest the necessity of higher regularity of the approximation of the flux map. But, enforcing continuity of the gradient of finite element functions on triangular meshes leads to a drastic increase in the number of unknowns, since the degree of the polynomial approximation needs to be increased beyond four. Therefore, existing implementations for the fixed-boundary problem resort to curvilinear quadrilateral meshes and approximation spaces based on cubic Hermite splines. Fine substructures in the realistic geometry of a tokamak, such as air-gaps, passive structures and the vacuum vessel prevent the use of quadrilateral meshes for the whole computational domain, as it would be necessary for the free-boundary problem.

In this work we propose a mortar method that employs two overlapping meshes, as firstly adopted in [2] in the context of eddy current non-destructive testing. One mesh with Cartesian quadrilaterals covers the vacuum domain and one mesh with triangles discretizes the region outside the vacuum domain. The two meshes overlap in a narrow region around the vacuum domain. This approach gives the flexibility to achieve easily and at low cost higher order regularity for the approximation of the flux function in the domain covered by the plasma, while preserving accurate meshing of the geometric details exterior to the vacuum. The continuity of the numerical solution in the region of overlap is weakly enforced by mortar projection.

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Eddy current testing models for the analysis of corrosion effects in metal plates

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Eddy current methods are often used in order to assess the effect of corrosion in metal plates [1]. In the present paper we analyze two direct models where a corroded sample (flaw) is replaced (for modeling purposes) by an inclusion of a cylindrical shape. A coil carrying alternating current is located above the conducting medium containing the inclusion. It is assumed that the axis of the coil coincides with the axis of the inclusion. In the first model the flaw is represented by the region of reduced electrical condutivity. The flaw in the second model consists of two layers. The upper layer contains air while the electrical conductivity of the lower layer is smaller than the conductivity of the surrounding medium.

The system of the Maxwell's equations in each of the regions is solved by the method of truncated eigenfunction expansions [2]. The formula for the change in impedance of the coil is derived. The obtained solution is quasi-analytical for the two reasons: (a) complex eigenvalues arising from the interface conditions where regions of different electrical conductivity are present have to be computed numerically and (b) the system of linear equations for the expansion coefficients also has to be solved numerically.

The change in impedance of the coil is computed for different frequencies of the excitation current and different parameters of the problems. The reduction of the electrical conductivity of the flaw on the change in impedance of the coil is investigated numerically. Recommendations for the solution of the inverse problems are presented.

The two models are also analyzed numerically using Comsol Multiphysics software. A finite element model is used for the computation of the change in impedance of the coil. Good agreement is found between computational results for the quasi-analytical and finite element models.

Keywords: eddy currents, truncated eigenfunction expansions, finite element modeling.
Acknowledgments. This work was partially supported by the grant 623/2014 of the Latvian Council of Science.

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Numerical simulation and optimization of induction heating in forge applications

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The objective of this work is to simulate and optimize the thermoelectric behavior of induction heating furnaces used for hot forging applications [3]. Namely, we are interested in heating steel cylinders which are used later to forge automotive parts. In order to determine the evolution of the temperature in the steel during the heating cycle we must solve a coupled thermal-electromagnetic model which takes into account the motion of the piece inside the furnace, and the fact that the material properties of the steel strongly depend on temperature. Taking into account the specific geometry of the furnace, we develop axisymmetric 2D and 1D models [1] and we compare the results obtained with both methodologies. The electromagnetic model, based on the eddy current approximation, is written in terms of the magnetic vector potential and is non-linear due to the ferromagnetic behavior of the steel. The thermal model includes the translational motion of the steel and computes the temperature in steady-state. The numerical solution of the coupled model is performed by means of finite element methods in the 2D-axisymmetric case and by means of finite difference approximations and ODE solvers in the one-dimensional case.

By using the numerical tools developed to simulate the furnace, we have used an optimization algorithm [2] to find optimum values of electrical frequency, current and velocity of the steel workpiece to raise the workpiece temperature to a specified level with a certain degree of uniformity. The optimization algorithm is based on the one-dimensional model which offers a good approximation of the 2D-model but requires much less computational effort. Thus, it is suitable for multiple evaluations of the objective function. We will present some numerical results corresponding to the simulation of an industrial furnace.

Keywords: induction heating, thermoelectric coupling, optimization, forge applications.

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Stability and convergence of fully explicit leap-frog DG scheme for solving 2D Maxwell's equations in anisotropic materials

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There are many materials whose optical properties depend on the direction of propagation. Among the cases in which optical anisotropy occurs; crystals and liquid crystals and photo-elastic effects we focus on a different and quite interesting case of optical anisotropy, form birefringence known as biological anisotropy. The form birefringence happens in most of the ocular tissues, namely retinal nerve fiber layer. In this work, we are interested in numerical solution of electromagnetic wave propagation in anisotropic materials which arise naturally in our application of interest [1].
Many recent papers on the simulation of electromagnetic waves propagation have shown interest in the use of discontinuous Galerkin time domain methods (DGTD) to solve Maxwell's equations. DGTD methods gather many desirable features such as being able to achieve high-order accuracy and easily handle complex geometries. Moreover, they are suitable for parallel implementation on modern multi-graphics processing units. Local refinement strategies can be incorporated due to the possibility of considering irregular meshes with hanging nodes and local spaces of different orders. Despite the relevance of the anisotropic case, most of the formulation of the DGTD methods present in the literature are restricted to isotropic materials. The treatment of anisotropic materials within a DGTD framework was discussed for instance in [3] (with central fluxes) and in [5] (with upwind fluxes).
Here we combine the nodal DG method [4], considering both central and upwind fluxes, for the integration in space with an explicit leap-frog type method for the time integration. We present a rigorous proof of stability and derive the error estimates for cases of typical boundary conditions (either perfect electric, perfect magnetic or first order Silver-Müller) [2]. Moreover a modified method is proposed to improve the order of convergence in time in the case of Silver-Müller boundary condition. The schemes stays explicit and stable with this modification in time integration. We illustrate the stability condition as well as the convergence order of the fully-discrete scheme, both in space and time for both type of fluxes and different boundary conditions with numerical tests.

Keywords: Maxwell's equations, Discontinuous Galerkin method, Anisotropic
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Thermo-electromagneto-hydrodynamic numerical simulation of the removal of volatile impurities in molten metals

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In this work a mathematical model is developed to investigate the removal of volatile impurities in a metal refining process. All the physical phenomena take place inside an industrial scale furnace.

The furnace essentially consists of a refrigerated stainless steel chamber containing a hemispherical crucible. The crucible and the molten mixture inside are heated by a heater, which is located below the crucible and connected to three-phase alternating current. Heat generated by the electric current, and transmitted mainly by radiation, keeps the metal contained into the crucible in liquid state. Eddy currents are induced into the melt leading to an electromagnetic force and thereby to a motion. Stirring and heating ensure the homogenization of the mixture and produce the vaporization of impurities that are condensed on the walls of a top chamber. Operating conditions in the chamber affect the kinetics of the process and the movement of the gases.

The overall process in the furnace is very complex due to the coupling of the different physical phenomena that take place: electromagnetism, heat transfer with radiation, motion in the molten and gaseous region, and chemical kinetics and thermodynamics of evaporation and condensation processes. On the one hand, the thermal mathematical model is coupled with the electromagnetic one because the Joule effect is a source terms in the heat transfer equation and the physical parameters depend on temperature. On the other hand, the dependence of the liquid buoyancy force on the temperature, the velocity in the convective term of the heat transfer equation and the electromagnetic force in the Navier-Stokes equation couple the hydrodynamic model with the others. Stirring and temperature distribution in the molten region determine the evaporation mass flow of the base metal and its impurities. Furthermore, this flow conditions the movement and distribution of gases in the condensation chamber. Finally, heats of reaction in the chamber walls and the convection generated by the gaseous movement should be incorporated into the global heat balance.

We state the partial differential equations and their corresponding boundary conditions modelling the overall 3D process and introduce a numerical algorithm for solving them. Finally, numerical results are shown. The results allow us to improve the furnace design and optimize its performance.

Keywords: Mathematical modelling, coupling, numerical simulation, metallurgy, impurities, refining.
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Topics in magnetic force theory: some avatars of the Helmholtz formula

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In eddy-current theory (where displacement currents and Coulomb forces are neglected), the force density is $J \times B + f$, where f is what is called here the 'magnetic force'. Let's assume a B–H law of the form $B = \mu H$, where μ may depend on the spatial position and on the density of the magnetic material. The classic Helmholtz formula is then (with many notational abuses):

$$f = -{}^1\!/_2 \, |H|^2 \, \nabla\mu + \nabla[\rho \, (\partial_\rho \mu) \, |H|^2/2], \tag{1}$$

to be understood in the sense of distributions (because of discontinuities of μ at material interfaces). This can be proved by using the Virtual Power Principle (VPP) [1], provided one knows the magnetic energy density $\psi_{\text{mag}}(x, b, \beta)$, as a function of position x, of the ambient induction b at this point, and of the matter's 'distortion' β (the linear map that describes how material points and material vectors are placed in physical space as the effect of a virtual motion).

A first difficulty, at this stage, is that ψ_{mag} is only a part of the total energy density $\psi(x, b, \beta)$ of the contraption, the other part being (let's address magneto-elasticity, for definiteness), $\psi_{\text{ela}}(x, \beta) = \psi(x, 0, \beta) = \psi(x, b, \beta) - \psi_{\text{mag}}(x, b, \beta)$. This splitting of the total energy density may look natural (the idea is that elastic behavior is insensitive to the magnetic situation), but one should be aware that a different splitting would lead to a different definition of f. Hence there are limits to the *objectivity* of the magnetic force concept: Force is well defined only *after* a magnetic compartment and an elastic one have been delimited in the magneto-elastic system under study.

This is not enough, however, to account for the bewildering variety of force formulas. For instance, one finds this in [2] (with a constant C):

$$f = C\rho\nabla(|B|^2/2), \tag{2}$$

which features a remarkable (and attractive, in many respects) proportionality of magnetic force with the gradient of magnetic energy. We'll see that such a formula *can* be derived from (1), but only under some restrictive assumptions that should not be overlooked. Otherwise, (2) is misleading.

Another example is about Kelvin's force, $f = M \cdot \nabla H$, when the B–H law is presented as $B = \mu_0 H + M$. This is commonplace in the study of ferrofluids [3]. Here, the derivation from the Helmholtz force relies on an additional hypothesis, namely the incompressibility of the fluid. First, suppose $\mathrm{rot} H = 0$ everywhere. Then $M \cdot \nabla H = \nabla H \cdot M$ (the so-called 'Maxwell force'). Comparing this with the Helmholtz expression, and assuming $\partial_\rho \mu = 0$ there, for the sake of simplicity, one finds that 'Kelvin' − 'Helmholtz' = $\nabla((H \cdot M)/2$, a gradient. If the ferrofluid is incompressible, one may apply the VPP to only those virtual velocities v such that $\mathrm{div} v$ = 0, and by integration by parts, the virtual power associated with the Kelvin and the Helmholtz expressions are then the same. So using Kelvin doesn't make a difference as regards the final solution of the coupled problem. Yet, as we shall argue, the 'Kelvin force' *is not the real force* in that case, and using it is risky.

Keywords: Helmholtz force, Kelvin force, ferrofluids.

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MS21: New developments in models of traffic and crowds

MS21: New developments in models of traffic and crowds

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Modern society is increasingly faced with problems arising from overcrowded and congested motorways, and control of large crowds (sometimes failing, resulting in casualties, even loss of life). Over-engineering or oversizing available space is not always an option, and there is a need for mathematically sophisticated solutions arising from dynamical systems modelling.

Recent studies have produced a number of detailed models for the many-body interactions that take place both in traffic flows (where vehicles ajust their motion and position of other vehicles) and in flows of crowds of pedestrians (where pedestrians ajust their motion to the motion and position of the sourrounding crowd). Classic and new mathematical techniques are brought to bear to study and describe the evolution dynamics: bifurcation theory, PDE and ODE reduction models, and equation-free analysis. The Minisymposium will explore current models, and models in development.

Speakers:

N. Forcadel, INSA de Rouen, France, *Justification of macroscopic traffic flow model by specified homogenization of microscopic models.*

N. García-Chan, University of Guadalajara, Spain, *Numerical Simulation of the Urban Pollution Related to Traffic Flow.*

J.-G. Caputo, INSA de Rouen, France, *A General Microscopic Trafic Model Yielding Dissipative Shocks.*

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M. P. Sørensen, Technical University of Denmark, *Emerging Traffic Jam Patterns in the Optimal Velocity Model for Traffic Flow.*

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

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The goal of this talk is to present and to justify Hamilton-Jacobi formulation for macroscopic traffic flow model. The idea is to show how it is possible to deduce macroscopic models of traffic flow from microscopic ones. The main advantage of microscopic models (in which we describe the dynamics of each vehicle in an individual way) is that one can easily distinguish each vehicle and then associate different attributes (like maximal velocity, maximal acceleration...) to each vehicle. It is also possible to describe microscopic phenomena like red lights, slowdown or change of the maximal velocity. The main drawback is for numerical simulations where we have to treat a large number of data, which can be very expensive for example if we want to simulate the traffic at the scale of a town.

On the contrary, macroscopic models consist in describing the collective behaviour of the vehicles for example by giving an evolution law on the density of vehicles. The oldest macroscopic model is the LWR model ([4, 5]), which dates back to 1955 and is inspired by the laws of fluid dynamics. More recently, some macroscopic models propose to describe the flow of vehicles in terms of the averaged spacing between the vehicles (in some sense, the inverse of the density, see the work [3]). The main advantage of these macroscopic models is that it is possible to make numerical simulations on large portion of road. On the other side, it is more complicated to describe microscopic phenomena.

Generally speaking, microscopic models are considered more justifiable because the behaviour of every vehicle can be described with high precision and it is immediately clear which kind of interactions are considered. On the contrary, macroscopic models are based on assumptions that are hardly verifiable. As a consequence, it is often desirable establishing a connection between microscopic and macroscopic models so to justify the latter on the basis of the verifiable modelling assumptions of the former.

The goal of this talk is to show how to pass from microscopic models to macroscopic ones. As we will explain, this problem can be seen as an homogenization result on a non-local Hamilton-Jacobi equation. More precisely, at the microscopic scale, we will consider a first order model of the type "follow the leader", i.e., the velocity of a vehicle depends only on the distance with the one in front of it and we will consider a local perturbation located at the origin which make slow down the vehicles. At the macroscopic scale, we attend to recover an Hamilton-Jacobi equation on the right and on the left of the origin and a condition of junction at the origin (as studied in [2]). This junction condition allows us to see the influence of the microscopic perturbation at the macroscopic scale.

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

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Numerical simulation of the urban pollution related to traffic flow

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The traffic flow is the main source of air pollution in urban zones. The cars are mobile sources and there are several thousands of vehicles in big cities and even millions in megacities. So, to estimate pollutant emission rates due to traffic flow is a very hard task. In this work, within the framework of mathematical modelling and numerical simulation, we propose a methodology for estimating the pollutant concentration on an urban domain. This methodology consists into combining a 1D traffic flow model with a 2D pollution model.

There are different mathematical models in partial differential equations (PDEs) for simulating the cars density on a road. One of the most referenced is the 1D first order model of Lighthill-Whitham-Richards (LWR). It is obtained from a conservation law, by assuming that flux and velocity depends only on the cars density (static relations). This model is very useful because it can be implemented on a road network with junctions, where the solution is guaranteed under certain hypothesis on the traffic flow (see [1]).

For simulating a city, we consider a 2D domain including the road network where the cars density can be obtained by the LWR model. To simulate the pollutant concentration we use a classical advection-–reaction—diffusion model (see [2]) and we propose to take into account the traffic flow contamination by including a source term proportional to the traffic flux on the road network. This flux is obtained by solving the LWR model and it is included in the 2D pollution model via a Radon measure supported on the network.

In this work we establish existence of solution for the no-coupled model conformed by the LWR model and the 2D pollution model, and we detail a complete algorithm to solve it: we combine the supply demand method (see [3]) for solving the LWR model with a characteristic Lagrange finite element method for the pollution model. Finally, we present some numerical experiments on a real urban domain: the Guadalajara city (Mexico).

Keywords: Traffic flux, air pollution, LWR model, mathematical modelling, numerical simulation
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A general microscopic trafic model yielding dissipative shocks

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Inspired by Aw and Rascle, we considered a general microscopic trafic model with a delay. For zero delay we prove that only a zero traveling wave solution exists. For a non zero delay, a formal derivation based on elliptic functions yields a traveling wave solution. The continuum limit of the model is a KdV-Burgers partial differential equation. Numerical simulations show indeed the dissipative shocks typical of KdV-Burgers. We also compare different structure functions and find traveling waves only for the "tanh" type. Algebraic structure functions yield an essential singularity. These results are compared to the ones obtained for other models and put into perspective.

Keywords: trafic models, asymmetric coupling, dissipative shocks

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Pedestrian dynamics from social force models

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Numerical simulation of pedestrians moving as mass points under the action of social forces and reacting to forces from obstacles provides a way to study crowd phenomenae. Increasingly, ensuring the safety of crowds at mass events, and in interactions with the built environment, relies on an understanding of the various collective states that a crowd may be in. Current social force models with inflexible parameters suffer from limited validity when they are applied to various scenarios. We present here a number of examples of this. We demonstrate typical pathological cases of unrealistic stationary points and show how it arises in models using potential forces. To overcome this problem we propose, and mathematically formalize, a novel hybrid modeling approach including dissipation via a friction term, where pedestrian behavior is situation-dependent, i.e., we switch between equations of motion according to the relative location to an obstacle. A new simulation framework, `ped->sim`, is introduced providing a straightforward implementation of these models. A number of scenarios are studied to illustrate the advantages of the new hybrid model approach.

Keywords: Crowd Dynamics, Social Force Models, Collective Phenomenae, Numerical Simulations.
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Analysis of unstable pedestrian flows

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A crowd evacuation scenario where pedestrians have to evacuate along a corridor by manoevering around an obstacle is investigated [1]. The route choice of each individuum, i.e. whether to go left or right around the obstacle, is influenced by the shortest path as well as by the walking pattern of the pedestrians in a neighborhood around the individual. This is investigated systematically by changing the position of the obstacle. Bistability and a hysteresis behaviour in the difference between fluxes on each side of the obstacle indicates the existence of an unstable pedestrian flow between the extreme cases where all pedestrians selected the same side of the obstacle. This parameter dependent behaviour and resulting qualitative changes are analyzed in detail.

Keywords: pedestrian flow, pedestrian model, particle model, hysteresis, bistability, bifurcation, macroscopic behaviour.

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Emerging traffic jam patterns in the optimal velocity model for traffic flow

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We present a car traffic model in the framework of the extended optimal velocity model where the driver can react not only to the preceding car but also to the following car [1]. Emerging periodic wave train solutions that describe the formation of traffic congestion patterns are found by numerical simulations. An understanding of the jam patterns as function of parameters is presented using a perturbation approach based on collective coordinates. The zero order equation for the perturbation method is the discrete modified Korteweg–de Vries equation, which possess soliton like solutions. We found analytical results that are in excellent agreement with full numerical solutions.

In the optimal velocity model a safety distance is included as a key parameter. Drivers tend not to drive closer than this specified safety distance. For cruise controls, which can adjust the car speed according to the speed of the preceding and the following car, a possible attempt could be to try applying a time modulation of the safety distance as a method for controlling the overall traffic flow. In particular this method may diminish the appearance of spontaneous traffic jams at high car densities [2, 3]. Indeed our simulations demonstrates the possibility of controlling traffic dynamics by applying high-frequency time modulation of the safety distance. It is shown that the region of the car density where the uniform (free) flow is unstable changes in the presence of time modulation compared with the unmodulated case. We shall discuss both periodic as well as stochastic time modulations of the safty distance and the ability to prevent or reduce formation of traffic jams.

Keywords: Traffic patterns, Optimal velocity model.
Acknowledgments. We acknowledge financial support from Civilingeniør Frederik Leth Christiansens Almennyttige Fond and the Otto Mønsted Foundation.

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MS22: Shape and size in biomedicine, industry and materials science: an ECMI special interest group

MS22: Shape and size in biomedicine, industry and materials science: an ECMI special interest group

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Statistical Shape Analysis, Stochastic Geometry, Mathematical Morphology and related disciplines deal with the geometrical information of families of objects in presence of stochasticity. Thanks to the development of information technologies, the last decades have seen a considerable growth of interest in the statistical theory of shape and its application to many and diverse scientific areas.

Often the diagnosis of a pathology, or the description of a biological process mainly depend on the shapes present in images of cells, organs, biological systems, etc., and mathematical models which relate the main features of these shapes with the correct outcome of the diagnosis, or with the main kinetic parameters are often still not present.

In material sciences and industrial applications optimization for quality control requires mathematical models from Stochastic Geometry and the related statistical estimation procedures, and methods of Statistical Shape Analysis and Mathematical Morphology for the description and comparison of different random geometrical patterns.

From the mathematical point of view, Shape Analysis and Stochastic Geometry use a variety of mathematical tools from differential geometry, geometric measure theory, stochastic processes, image analysis, etc., dealing with both direct and inverse problems.

As far as applications are concerned, in this minisymposium topics which are relevant in biomedicine and material sciences will be emphasized.

This is a minisymposium of an ECMI Special Interest Group which originated about 14 years ago from a working group of the Network of Excellence MACSInet and is now continuing its activities with the support of ECMI. This ECMI SIG has been very active along the years, organising regular workshops, minisymposia and meetings with presentations of current problems by "Industry" and/or of current methods by "Academia". Scientific collaboration and research projects among the members are active and encouraged.

A web page with a description of the activities of the ECMI-SIG can be found at http://www.mat.unimi.it/users/shape/.

Speakers:

M. Longfils, Chalmers University of Technology (Sweden). *Generalised Eden growth model and random planar trees.*

S. Velasco Forero, Mines ParisTech (France).*Hierarchical analysis of signals on graphs.*

A. Micheletti. Università degli Studi di Milano (Italy). *Statistical properties of the estimators of parameters of a germ−grain model for dual phase steel.*

H. Wang, Mines ParisTech (France). *Modeling of the microstructure of mesoporous alumina constrained by numerical simulation of nitrogen porosimetry.*

P. Easwaran, ITWM Kaiserslautern (Germany). *Stochastic modeling of 3D fiber systems incorporating interaction.*

J. Angulo, Mines ParisTech (France). *Morphological semigroups and scale−spaces on ultrametric spaces.*

G. Naldi, Universitá degli Studi di Milano (Italy).*Around the image analysis of the vessels remodelling during embryos development.*

Keywords: Mathematical morphology, Stochastic Geometry, Image analysis, Biomedicne, Material Sciences.

Generalised Eden growth model and random planar trees

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We study the Generalised Eden model on the integer 2D lattice which is a graph G with the nodes $\mathbb{Z}^2$ and edges drawn between all pairs of nodes at the distance 1 from each other. It is a growth process which is described as follows. A *crystal* is a connected subset of $\mathbb{Z}^2$, its nodes are called *occupied*, the nodes at the distance 1 of the crystal are called the *boundary nodes*, all the other nodes of $\mathbb{Z}^2$ are called *empty*. Let ξ_t be a crystal observed at time $t = 0, 1, \dots$. At every next time step $t + 1$ a boundary node x of ξ_t *crystallises* to form crystal $\xi_{t+1} = \xi_t \cup \{x\}$. The boundary node to crystallise at each step is chosen randomly with the probability depending on the number of already crystallised neighbouring nodes: if $N(x)$ denotes the set of neighbours of the point $x \in \mathbb{Z}^2$, then the probability that x crystallises at time $t + 1$ equals

$$\frac{r(|N(x) \cap \xi_t|)}{\sum r(|N(y) \cap \xi_t|)},$$

where the sum in the denominator is over all y in the boundary of ξ_t and $r : \{1, 2, 3, 4\} \mapsto \mathbb{R}_+$ is a *rate function*. The classical Eden model is obtained by considering a linear function r.

We focus on the limiting behaviour of the crystal. For the case of a growing r, it is known that there exist a compact set (a *limiting shape*) to which the normalised crystal $\xi_t/\sqrt{t}$ converges in the Hausdorff metric as $t \to \infty$, although in general little is known about the shape. A real challenge represent the case of non monotone rates r where all existing methods used to prove the shape result, in particular, the subadditivity property, fail. We study the most extreme case with the rates given by $r(1) = 1,\ r(2) = r(3) = r(4) = 0$ which produces a crystal without loops, i.e. a random tree, and we call it a "flake process". Even in this case, computer simulations shows that there exists a limiting shape, but a rigorous result or even tools to prove it are still missing. Another intersting feature of the flake process is existence of *holes* which are empty nodes 'inside' the crystal which will never get crystallised. We prove that the distibution of a hole size decays at least exponentially, implying that if a limiting shape does exist, it is necessarily one-connected.

Keywords: Eden model, random tree, asymptotic shape.
Acknowledgments. Financial support from the Swedish Foundation for Strategic Research, SSF, and Knut and Alice Wallenberg Foundation, KAW, is highly appreciated.

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Hierarchical analysis of signals on graphs

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Graph-based techniques on signal processing using a generic data representation which are useful for describing geometric structures including images, videos, 3D mesh objects, and network data as social network, geo-referenced data and many more [1]. The main idea is to model data structure by means of an affinity graph where each edge encodes the similarity among pairs of elements in the data set. For the case of images, the affinity graph includes a pixel-wise gradient which encodes local differences in the spatial domain. This simple but general framework allows to formulate many image processing and data analysis problematics including:

(1) *Hierarchical network simplification*, which carries out a multiscale simplification of the original dataset, in the sense of hierarchical clustering. The flexibility of our formalism make easier the inclusion of prior information about the characteristic of the desired clusters. Advantages of our formulation are illustrated in the case of hierarchical segmentation in the morphological sense, against state-of-the-art methods [2, 5].
(2) *Network regularization*, where one can find some works about nonlinear filters on graphs, particularly mathematical morphology operators in the algebraic sense [3, 4], where the couple of nonlinear operator (dilation/erosion) are maps for graph-valued signals, i.e., they are maps "from nodes to nodes". This approach allow us to extract structures in different scales, meaning components associated to shape/size features of the analyzed objects. Results of our approach are illustrated in mesh-valued data, and application to pattern recognition are also considered.
(3) *Semisupervised graph-based classification*, which is formulated as an energy function minimization, where the target function to estimate is smooth with respect to the underlying graph structure. Seed-based segmentation becomes then a labeling problem than can be solved by graph-based learning methods [6]. A comprehensive set of quantitative and qualitative comparisons against state-of-the-art algorithms that shows the effectiveness of our method.

The goodness of our procedure is illustrated from theoretical and practical points of view, including recent industrial projects about simplification and classification of hyperspectral image, classification and retrieval of objects via 3D+depth sensors and hierarchical simplification of manifold-valued images.

Keywords: Graph signal processing, Hierarchical data analysis, Hierarchical image processing, Mathematical Morphology.
Acknowledgments. This work has been partially supported by the Eureopean Union under *M3S project*.

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Statistical properties of the estimators of parameters of a germ-grain model for dual phase steel

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In many industrial or materials science applications the stochastic geometry of a real sample can be well approximated by a germ-grain model [1, 2]. A germ-grain model is composed by an overlapping of *germs*, that is elements of a point process in $\mathbb{R}^2$ or $\mathbb{R}^3$, each surrounded by a *grain*, that is a random closed set with a given distribution. Depending on the probabilistic structure both of the point process of germs and of the grains, the resulting model can be very complicated, so that it is very difficult to apply classical methods for parameter estimation, like e.g. maximum likelihood. In such cases parameters are estimated by minimizing a suitable distance between some geometric characteristics measured on real samples of the material under study and on computer simulations of the germ-grain model which must be fitted to real data. In such situation the statistical properties of the estimators can be studied with empirical procedures, starting from a simulated sample with known parameters, and comparing the results of many parameter estimations with the true values. Here we will present the results of a study of this kind applied to a germ-grain model which proved to be a good geometrical model for a sample of dual phase steel provided by Nippon Steel & Sumitomo Metal [3, 4, 5]. The model was fitted by using about 150 sections of a ferrite-martensite steel sample. Since the experimental costs to obtain images of sections of steel samples are very high, one important industrial problem is to reduce the number of 2D sections needed to reconstruct or simulate in a realistic way the 3D geometry of the material. This reduction causes an expected increase of the uncertainty in the parameters estimate of the fitted germ-grain model. The study of the statistical properties of the parameters estimators may help in quantifying the increase in uncertainty.

Keywords: germ-grain model, parameters estimation, dual phase steel, uncertainty quantification
Acknowledgments. This work has been partially supported by Nippon Steel & Sumitomo Metal and by the funds for research improvement from Universitá degli Studi di Milano.

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Modeling of the microstructure of mesoporous alumina constrained by numerical simulation of nitrogen porosimetry

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A procedure is proposed to simulate numerically experimental capillary condensation and evaporation isotherms in porous media, and to simulate random microstructures based on such isotherms. The present methodology is applied to a mesoporous material made of nanometric alumina "platelets".

First, a numerical method is developed to compute the adsorption and desorption isotherms in digital porous media. The method, based on simple morphological operators, extends that of Münch and Holzer [1] on mercury porosimetry. The meniscus of the vapor-liquid interface occurring during adsorption are simulated using a closing of the solid phase by a sphere. The diameter of the sphere controls the radius of curvature of the vapor-liquid interface. To simulate desorption, a combination of closing and hole-filling operators is used. For random media, the desorption curve is strongly sensitive to the volume of the computational domain. We overcome this effect by a percolation analysis of the gazeous phase during desorption. The present method allows one to predict the hysteresis and pore size distribution associated to porosimetry. To validate this approach, numerical results on simple geometries are compared with the work of Štěpánek et al. [2] based on the Kelvin equation.

Second, the condensation and evaporation isotherms occurring in various ideal Boolean models are computed and interpreted. In these models, the solid phase is made of spheres, prolate or oblate cylinders. Then, we study various two-scale models made of intersections and unions of Boolean models of spheres and cylinders. The multiscale microstructures exhibit an important hysteresis, contrary to their one-scale counterpart.

Third, nitrogen porosimetry data for mesoporous alumina is considered. Based on results obtained for multiscale microstructures, a random model is proposed for mesoporous alumina. To control both the size distribution and hysteresis, the porosity is made of a union of Boolean and hard-core models of spheres. The parameters of the model are identified and numerically adjusted to reproduce the experimental isotherms. Finally, we develop a model of mesoporous alumina made of aggregates of locally-aligned alumina platelets, as introduced in a previously-developed model [3]. The model contains the following characteristic scales: the platelets's size, that of platelets aggregates, and the size-distribution of pores.

Keywords: Capillary condensation; Porosimetry; Adsorption; Random model; Pore size distribution

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Stochastic modeling of 3D fiber systems incorporating interaction

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Non-woven materials are widely used in automotive industries to manufacture oil filters and air filters. The micro-structure of the non-woven materials significantly influences the efficacy of the filters. Realistic 3D micro-structure models for these materials are required for effective simulation of macroscopic filter properties. Altendorf and Jeulin [1] developed a realistic stochastic model for the fiber component in glass fiber reinforced composites. Since non-woven fibrous materials prominently feature fiber bundles, in this work, fiber bundles are introduced into the Altendorf and Jeulin model. To this end, fiber bundles are incorporated in the overlapping fiber system serving as starting configuration of the model. Then, the force biased fiber packing approach is applied to remove any overlap from the system, i.e., render the fiber system non-overlapping while keeping the fibers intact. The essential model parameters are fiber volume density, distribution of fiber diameter, orientation and length, a parameter for fiber bending, frequency of fiber bundles and number of fibers in each bundle. These parameters need to be estimated from the real data for model fitting. The fiber volume density is easily calculated from the binarized image of the fiber system. The algorithm based on directed distance transform developed in [2] can be applied to compute the fiber diameter distribution. The global fiber orientation distribution is assumed to follow the distribution [3] which is a special case of the angular central Gaussian distribution. We estimate the anisotropy parameter of this distribution following [4, 5]. The single fiber separation approach based on probability maps developed in [2] can be used to estimate the fiber length, and the parameters for fiber bending and for fiber bundles. In order to avoid the error-prone individual fiber segmentation, local curvature estimation as proposed in [6] is explored as an alternative for estimation of the fiber bending parameter.

Keywords: Fiber system model, Fiber bundle, Image analysis, Fibrous media, Non-woven.

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Morphological semigroups and scale-spaces on ultrametric spaces

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Morphological semigroups for functions on length spaces have recently studied [2], whose basic ingredients are the convolution in the $(\max, +)$-algebra (or supremal convolution), the metric distance and a convex shape function. Links with Hamilton–Jacobi PDE on length spaces appears also naturally. These semigroups lead to powerful scale-space properties for multiscale filtering, regularization and feature extraction. Such operators on length spaces endowed with a Maslov measure are also related to idempotent analysis [3]. The goal of this paper is to consider a similar generalization of morphological semigroups to the case of functions on ultrametric spaces.

Every finite ultrametric space is known to admit a natural hierarchical description called a dendogram. Dendrograms represent a tree structure of the data, where the data points are the leaves of the tree and the vertical axis reveals the ordering of the objects into nested clusters of increasing ordering: subsets of data points are clusters represented by the internal vertices, and inclusions of clusters are represented by paths between the corresponding vertices. We can define an ultrametric distance between two points of such set of leaves as the minimal number of steps (internal vertices) one should go up the dendogram to find a common ancestor of the two points.

Datasets endowed with a hierarchical classification structure are nowadays used in many applications and challenging problems in industrial mathematics; that can be the case of very high dimensional spaces where the data structure is generally given by cluster-like organization. In the case of morphological image processing, hierarchical representation are ubiquitous. Processing a function whose domain is such hierarchical representation requires the formulation of filters and operators on ultrametric spaces. The counterpart of Heat kernel and Heat semigroups on ultrametric spaces has been widely studied in recent work [4] and consequently, using this theory all diffusion-based signal/image processing techniques can be applied to filter out functions on a hierarchy. A similar counterpart of morphological signal/image processing for such representations is developed.

Our starting point is the notion convolution of two functions in the $(\max, \min)$-algebra. Using this operator, we have recently shown that morphological operators on Euclidean spaces are natural formulated in $(\max, \min)$-algebra [1]. We introduce $(\max, \min)$-convolution based morphological operators on ultrametric spaces, where the structuring functions are scaled versions of the ultrametric distance (raised to a power $p \geq 1$). We study the corresponding semigroups properties and illustrate their interest in filtering and feature extraction. The equivalence with the solutions of a particular family of Hamilton–Jacobi PDEs is also considered.

Keywords: ultrametric space; mathematical morphology;
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Around the image analysis of the vessels remodelling during embryos development

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The cardiovascular system is the first organ system to develop and reach a functional state in the mammalian embryo. This reflects the crucial need for a vascular supply for the delivery of nutrients and the disposal of catabolic products from normal tissues. The blood vessels that initially comprise this organ originate by vasculogenesis, the aggregation of de novo-forming angioblasts (endothelial precursors) into simple endothelial tubes [1]. Given the complex nature of the vascular system and the diversity of biological processes required for its assembly and refinement, it is hardly surprising that a large number of signalling pathways are employed in its development. Mutations in pathways required for vascular development frequently manifest phenotypes that result in embryonic lethality at mid gestation. The vascular activities of these pathways are not limited to this developmental time window, but extend to organogenesis, maintenance of vascular homeostasis in adulthood and states of pathological angiogenesis. Here, we focus on the role of the semaphorins cues in the early vasculature process [2]. In particular, we develop a suitable image analysis tool in order to detect and classify vasculature impairs due to the inhibition of semaphorin $3A$ in mice embryo starting from confocal microscopy images [4].
Two criteria that have been proven to be useful for a human-made identification of this hierarchical structure are: long, thick and almost aligned branches near the center of the head, with long and narrow holes in between; more fine-grained network in the external area, with thinner vessels and well-defined holes. In order to analyze these features, we consider the shape and the distribution of the "holes" formed by the vascular network. The high variance in the intensity of the image makes it impossible to find a global background/foreground threshold to identify the whole topology of the vascular network. Moreover, the noise and the local characteristics of the image are such that it is difficult to find a general method to identify suitable local thresholds. In fact, both the bigger vases and the background of the image show strong irregularities, that cause many standard methods to incorrectly identify holes where only darker portion of vases are, and portions of vases in place of background noise [1].
A custom combination of a global and a local approach has then been found to obtain a binarization of the image, and segment it. Three features and the distributions of the holes have been studied: size of the hole; elongation and alignment with the vertical axes; approximate distance from the center of the head. These measures have some limitations, as for some precision issue on the distance calculation, but they already showed good preliminary results without further refinements.

Keywords: Vascular plexus formation, Segmentation, Network patterns, Impaires detection.
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MS23: Charge transport in semiconductor materials: emerging and established mathematical topics

MS23: Charge transport in semiconductor materials: Emerging and established mathematical topics

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Modern electronic devices would be unthinkable without semiconductor materials. Few inventions have shaped our modern society like they have. There are emerging fields such as organic semiconductors, where there is still the demand to develop models and new theory, and there are many well-established fields, e.g. particle detector simulations, where it is mostly required to develop advanced numerical methods.

The aim of this mini symposium is to encourage communication between both worlds, applied mathematics (or industrial mathematics) and the field of fundamental research on numerical methods, mathematical modeling, and optimal control problems related to semiconductor (charge transport) models.

Speakers:

René Pinnau. TU Kaiserslautern, Department of Mathematics (Germany). *Combining Asymptotic Analysis and Optimization in Semiconductor Design.*

Patricio Farrell. Weierstrass Institute Berlin (Germany). *Scharfetter-Gummel Schemes for Non-Boltzmann Statistics.*

Klaus Gärtner. Università della Svizzera italiana, Institute of Computational Sciences (Italy). *Takahashi formulas and the generalized Takahashi structure.*

Matthias Liero. Weierstrass Institute Berlin (Germany). *On $p(x)$-Laplace thermistor models describing electrothermal feedback in organic semiconductor devices.*

Victor Burlakov. Mathematical Institute, OCCAM, Oxford (UK). *Multi-Scale Kinetics of Photo-Excited Charges in Organo-Lead Perovskites.*

Wil Schilders. TU Eindhoven (Netherlands). *Numerical methods for the simulation of organic and anorganic.*

Axel Fischer. Institut für Angewandte Photophysik, TU Dresden (Germany). *Multi-physics simulation of organic devices using LTspice for first principle understanding.*

Matthias Auf der Maur. University of Rome Tor Vergata, Rome (Italy). *Multiscale approaches for electronic device simulation.*

Dirk Peschka. Weierstrass Institute Berlin (Germany). *Toward the optimization of Ge microbridges.*

Combining asymptotic analysis and optimization in semiconductor design

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Keywords: Asymptotic analysis, model hierarchy, semiconductor design, optimization

We present the quasi-neutral limit in an optimal semiconductor design problem constrained by a nonlinear, nonlocal Poisson equation modelling the drift diffusion equations in thermal equilibrium. While a broad knowledge on the asymptotic links between the different models in the semiconductor model hierarchy exists, there are so far no results on the corresponding optimization problems available. Exploiting the variational structure of the problem, we end up with a bi-level optimization problem, which is thoroughly analysed. Using the concept of Γ-convergence we perform the quasi-neutral limit for the minima and minimizers. This justifies the construction of fast optimization algorithms based on the zero space charge approximation of the drift-diffusion model.

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Scharfetter-Gummel Schemes for Non-Boltzmann Statistics

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When modelling semiconductor devices via the van Roosbroeck system one often uses statistical distribution functions to describe the correspondence between carrier densities and chemical potentials. For 3D bulk semiconductors this is achieved by the Fermi-Dirac integral of order $1/2$. Frequently, one approximates it with a Gaussian (Boltzmann approximation). Already in the late 60s, Scharfetter and Gummel suggested a numerical scheme to deal with the numerical challenges posed by the van Roosbroeck system using the Boltzmann approximation [1].

However, how to numerically solve the van Roosbrock in the general case of non-Boltzmann statistics is still an open problem [3]. We will present several methods to generalise the Scharfetter-Gummel scheme [2, 4, 5]. Our main goal is to discretely preserve important properties from the continuous system such as existence and uniqueness of the solution, consistency with the thermodynamical equilibrium and unconditional stability. We also show how these numerical methods can be efficiently implemented for 2D and 3D applications.

Keywords: semiconductor devices; finite volume method; Scharfetter-Gummel scheme; thermodynamic consistency.

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Takahashi formulas and the generalized Takahashi structure

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Computing selected elements of the inverse of a structural symmetric sparse matrix A can be done efficiently for the sparse subset Z by the Takahashi recurrence. The computational complexity is that of the LU factorization for A. The technique can be extended to treat the three factor product

$$X = A^{-1}YB^{-1},$$

where A, Y, B are given sparse matrices with some additional properties. Special cases of interest are $B = A^T$, the congruence transformation (e.g. quantum physical evolution processes described by the NEGF techniques) or $B = A$, describing the parameter dependence of the inverse with respect to parameters p_i entering A ($y_{ijk} = \frac{\partial a_{ij}}{\partial p_k}$). We give an explicit prove that X can be computed by Takahashi like techniques with the complexity of the LU factorization of A.

Based on the proof special aspects of the related algorithm, especially its parallelization, will be discussed. The algorithm will be made available via the sparse linear solver PARDISO.

Keywords: sparse matrices, computation of selected elements of the inverse, quantum scattering problem, sensitivity of the inverse matrix.

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On $p(x)$-Laplace thermistor models describing electrothermal feedback in organic semiconductor devices

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Organic semiconductor devices are thin-film multilayer structures consisting of organic, i.e. carbon-based, molecules or polymers. Nowadays, they can be found in everyday life in smartphone displays, photovoltaic cells, and TV screens. In addition, organic light-emitting diodes (OLEDs) have been identified as a promising alternative to conventional solid-state lighting.

However, several technological issues in the development of efficient large-area OLEDs exist. In lighting applications, a much higher brightness than in displays is required. At high power, a substantial self-heating in the device occurs, which leads to unpleasant brightness inhomogeneities. Although the role of electrothermal interplay has been recognized, the fundamental understanding of this mechanism is still missing. For example, there is no explanation why the highest temperature is reached at the device boundary although the heat conduction is worst at the center of the structure. Furthermore, lighting panels can show a saturation of brightness around their center at elevated self-heating, see [1].

In this talk, we present analytic results for a new stationary thermistor model, introduced in [2], to describe the electrothermal behavior of large-area OLEDs ([3, 4]). The coupled system consists of the current-flow equation for the electrostatic potential and the heat equation with Joule heating term as source. The self-heating in the device is modeled by an Arrhenius-like temperature dependency of the electrical conductivity. The non-Ohmic electrical behavior of the organic material is described by a power law such that the electrical conductivity depends nonlinearly on the electric field. Notably, we allow for functional substructures with different power laws, which gives rise to a $p(x)$-Laplace-type problem with piecewise constant exponent.

The talk presents joint work with M. Bulíček (Charles University Prague), A. Glitzky and T. Koprucki (WIAS) and reports on experimental results of A. Fischer and R. Scholz (Institute of Applied Photophysics, TU Dresden).

Keywords: Thermistor problem, $p(x)$-Laplacian, organic semiconductor, Arrhenius law.
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Multi-scale kinetics of photo-excited charges in organo-lead Perovskites

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Multiple photoluminescence (PL) studies of Methyl-Ammonium Lead Halide Perovskite (MALHP) have revealed numerous mechanisms affecting the relaxation of the photo induced charge carriers and acting on different time scales from nanoseconds to minutes. We present a model accounting for such multi-scale evolution of PL intensity. The main and the quickest mechanism in our model is active on the time scale of 10-100 nanoseconds and is a non-radiative electron-hole recombination mediated by deep electronic traps, supposedly halide vacancies. This competes with bimolecular recombination of free electrons and holes, which is predominantly radiative. The concentration of the traps involved in such Shockley-Read-Hall recombination is in turn affected by the formation of the electron-trap complexes stable on the time scale up to fractions of a second. Furthermore, the concentration of the traps, or the vacancies, can generally depend on the ambient conditions and even can depend upon illumination. This variation is likely to occur on the time scale of seconds, or even minutes. To characterise each of the above mechanisms we analyse the time evolution of the PL intensity on the appropriate time scale and fit it with a suitable model function. The intermediate time scale of the charge carrier evolution in our model is determined by the recombination rate constant of the trapped electrons with free holes. It can be characterised by analysing the response of PL intensity under continuous illumination to a small change in the excitation intensity. The slowest evolution of the PL intensity taking place on the scale of minutes is explained by a variation of the trap concentration under continuous excitation. The model allows thorough characterization of both charge carriers and point defects kinetics in the perovskite material hence, helping us understand potential avenues towards improving its photovoltaic properties.

Keywords: carrier recombination, point defects, defect kinetics

Numerical methods for the simulation of organic and anorganic semiconductor devices

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The semiconductor device problem has been one of the hardest problems to solve numerically. To date, the drift-diffusion model, consisting of three coupled partial differential equations for the electric potential and the quasi Fermilevels, is still the most used model due to its accuracy when using advanced models for the mobility and reecombination paramaters. When analysing the model mathematically, it turns out that the equations are singularly perturbed, with a very small parameter. This parameter corresponds to what is known in physics as the Debye length. Besides the singularly perturbed character, the problem is also extremely nonlinear, and satisfies maximum principles that guarantee positivity of the carrier concentrations (electrons and holes). Furthermore, a number of conservation properties can be established.

Because of the aforementioned properties, the drift-diffusion equations are very hard to solve numerically, especially if one aims at robust and efficient methods that work for all possible devices: diodes, MOS transistors, bipolar transistors, FINFETs, thyristors. Standard numerical methods fail: finite difference methods do not satisfy the current conservation property, and standard finite element or finte volume methods cannot cope with the singularly perturbed character. The extreme nonlinearities result in non-convergent Newton processes, overflow and other convergence problems.

By now, however, robust and efficient techniques have been developed that can also be an inspiration for other fields, as they are sufficiently general in nature. In this presentation, we will discuss some of these techniques, and reflect on the background of their development. Besides the semiconductor devices commonly used in electronic circuitry, we will also touch upon the simulation of organic devices suchas OLEDs, for which simulation methods are quite related.

Multi-physics simulation of organic devices using LTspice for first principle understanding

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Simulation tools are nowadays frequently used to study complex scientific problems. For standardized problems, a wide range of commercial software exists. However, if new phenomena have to be investigated new tools must be developed or purchased which hinders a direct and prompt modeling of the experimental results. Here, we discuss the use of the freely available circuit simulator LTspice (http://www.linear.com/designtools/software/) as an efficient tool to quickly create models giving a first principle understanding. On the basis of this approach, we will present some recent issues in the field of organic electronics.

The electrothermal feedback in organic light-emitting diodes (OLEDs) is one challenging topic [1]. These devices are extremely thin ($\sim$ 100 nm) but expand over hand-sized areas, resulting in a huge aspect ratio. Having a thermally activated conductivity, OLEDs tend to show a strong positive feedback between the current flow and the power dissipation [2]. Such a behavior is described by thermistors having an "S"-shaped current-voltage characteristic under steady-state condition and can be excellently modeled by equivalent circuits implemented in LTspice. By that, extended resistive networks for the electrical as well as the thermal part are generated by a script, further connected by an 2D array of thermistor devices. The simulation reveals the lateral propagation of a region having a local negative differential resistance. Furthermore, so called "switched-back" regions and a new switching phenomenon for special electrode designs are revealed, giving a first insight to the complexity of the problem.

Such a network model is also helpful to understand the lateral current flow in OLED structures having a sandwich-like layer structure. Due to highly doped layers, light emission occurs outside the overlap area of the crossbar electrodes. The light emission in the metal-free area is of great interest for fully transparent OLEDs and future lasing applications.

A third issue are contact resistances in organic field-effect transistors (OFETs). Here, we use a laterally expanded network of resistors with a nonlinear current-voltage characteristic to phenomenologically model the charge injection and transport in the source and drain region. As an outcome, we are able to resolve the laterally expanded charge injection, helping to optimize the device structure regarding highest switching speed and minimum usage of footprint area.

Finally, the knowledge gained by the simulation with LTspice can be the basis for the development of more sophisticated tools which perfectly suit a particular problem.

Keywords: Circuit simulator, Organic light-emitting diode, Electrothermal feedback, Equivalent network model, Organic field-effect transistor
Acknowledgments: This work was financed by the European Community's Seventh Framework Programme under Grant Agreement No. FP7-267995 (NUDEV). Support from the excellence cluster cfaed is gratefully acknowledged. We thank the German Academic Exchange Service (DAAD) for a conference travel grant.

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Multiscale approaches for electronic device simulation

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Multiscale approaches for the simulation of semiconductor devices have been gaining increasing importance during the last decade. On the one hand, coupling of continuous media with particle based models are of interest for ultra-scaled electronic devices and for nanostructured light emitting and photovoltaic devices, both based on inorganic and organic materials, in order to resolve important microscopic details of the device structures. On the other hand, there is a need to combine microscopic transport models like Monte Carlo, density matrix based or non-equilibrium Green's functions (NEGF) with semi-classical ones like drift-diffusion in order to comprehensivley describe the macroscopic behaviour of devices with nanoscale active regions.

Modeling the transport of charge carriers or heat in downscaled devices requires the use of microscopic models including quantum mechanical and non-equilibrium effects. However, nanometer sized active device regions addressed by such models are usually embedded in larger environments, which influence device behavior in multiple ways. An overall device simulation should therefore be able to capture these details, particularly in view of device optimisation which more and more must go towards the physical limits of the available technology. Since microscopic quantum-mechanical models cannot usually be used on the whole device structure for computational reasons, especially if based on an atomistic description, and since the embedding regions are often well described by efficient semi-classical models, multiscale approaches become necessary [1, 2].

Having an application oriented use of multiscale models in mind, we will illustrate different ways of integrating transparently simulation models on different scales in a multiscale/multiphysics simulation environment. Results of parametric coupling between semi-classical and atomistic descriptions will be shown, which can give detailed insight into measurable device quantities hidden to standard continuous media models [4]. Approaches to concurrent coupling of NEGF with drift-diffusion present in literature will be discussed[5, 6], and current work towards integration of kinetic Monte Carlo or master equation based approaches with finite element based drift-diffusion, which is interesting for organic devices, will be illustrated.

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Towards the optimization of Ge microbridges

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Silicon photonics has become a rapidly developing new field with a high potential for low-cost solutions to problems ranging from high-speed data transfer for optical on-chip communication to bio-sensing. Beside successful demonstrations of the capabilities of this technology platform, the missing piece in the *silicon photonics toolbox* is believed to be a monolithically integrable active light source compatible with silicon technology. To fill this gap different concepts based on silicon (Si) and germanium (Ge) are under consideration, cf. e.g. [1]. The pioneering work in this direction is the successful demonstration of an electrically pumped laser based on slightly tensile-strained Ge/Si heterostructures by MIT researchers [2]. The extremely high lasing threshold currents observed in these devices lead to strong heating effects limiting their operation lifetime. This shows the strong demand for improvements, in particular, for rigorous optimization of Ge-semiconductor lasers.

We discuss two different approaches to fulfill this demand. On the one hand, a shape optimization with respect to material distribution in order to reach high strains and as a result reach higher gain due to the reduced direct band-gap. On the other hand, a doping optimization as in [5] to further increase optical gain and minimize optical losses by simultaneously solving the charge transport in a semiconductor. Heuristic case studies from [3, 4] are used in order to motivate the cost functionals used in the optimization.

Keywords: semiconductor, optimization, laser

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MS24: Masters in industrial mathematics. Overview and analysis of graduates and business collaborators

MS24: Masters in Industrial Mathematics. Overview and analysis of graduates and business collaborators.

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To educate in Industrial Mathematics is one of the main objectives of ECMI. In the past editions of the ECMI conferences the different training opportunities offered by institutions have been analyzed.

The aim of this Minisymposium is to propose a space for debate in which those responsible for the different titles in Industrial Mathematics can share with researchers in the field the new contributions that are being offered on the international scene.

We suggest that presentations deal with the visions graduates have once their education is over and they enter the working world. Moreover, in many of these qualifications companies collaborate as teachers, internship tutors and suggesting master dissertations. We think it is extremely important to share and analyze the opinions of graduates and companies under the ECMI umbrella as we believe collaboration in industrial mathematics is so Important.

Speakers:

T. Kauranne. Lappeenranta University of Technology (Finland). *International and double degree master studies and industrial collaboration in Technomathematics: a Finnish-Russian-African-Indian perspective.*

E. Lindner. Institute of Computational Mathematics, Johannes Kepler University Linz (Austria). *Technical mathematics and industrial mathematics at Johannes Kepler University Linz (JKU).*

O. López-Pouso, Department of Applied Mathematics, Universidade de Santiago de Compostela (Spain). *ECCUM, the creation of a Central Asian MSc with European cooperation.*

W. Okrasiński. Faculty of Pure and Applied Mathematics, Wrocław University of Technology (Poland). *Interdisciplinary approach to the mathematical modelling in a high school – an example from Poland* .

E. Vázquez-Cendón. Department of Applied Mathematics, Universidade de Santiago de Compostela (Spain). *Master in Industrial Mathematics (M2i). Learning 4.0 cross-institutional education to solve real problems in industry.*

S. Abreu. Department of Mathematics, Polytechnic of Porto and LEMA, Laboratory for Mathematical Engineering, Porto (Portugal). *The Master of Applied Mathematics to Engineering and Finance of the School of Engineering, Polytechnic of Porto, Portugal.*

T. Mendonça. Departamento de Matemática, Faculdade de Ciências da Universidade do Porto (Portugal). *The Master degree of Mathematical Engineering at the University of Porto.*

J. A. Ferreira. CMUC, Department of Mathematics of University of Coimbra, (Portugal). *Training mathematician in the University of Coimbra: an ECMI master program.*

Keywords: Masters in Industrial Mathematics, graduates, business collaborators

International and Double Degree Master Studies and industrial collaboration in Technomathematics: a Finnish-Russian-African-Indian perspective

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International collaboration in Technomathematics and other fields of Higher Education can take many forms. Universities with strong brands and historic credentials can hope to attract a lot of international students even if they charge high term fees. Many universities in Europe have been established primarily to provide higher education for a large number of domestic students and face a new and challenging situation in addressing the ever more global market for education and scientific collaboration. One of the first hurdles that needs to be tackled is the need for a balance between providing a sound basic education in each discipline providing a degree programme, and the need to reach excellence in some crucial sub-fields. A second major issue is the demography of the ever more global student population.

The Applied Mathematics program at Lappeenranta University of Technology was initially set up just to provide basic calculus courses for engineering BSc students. Ambition and dearth of students majoring in Maths made us turn to the international student market with the twin assets of a focus on Technomathematics and free tuition. Lack of a recognized brand led LUT to approach universities abroad through personal contacts between like-minded professors, for which ECMI has proven an excellent vehicle. The emergence of Eastern Europe and Russia from the limitations of the Cold War provided a nearby market of curious, motivated and talented students. The best way to learn to know them was to travel as a guest lecturer to their home universities, as well as inviting professors from these countries to deliver special courses to our own student body. That encouraged visiting professors to send their students to enrol in the LUT Master programme, and later on to imitate the ECMI curriculum in their own university and establish a Double-Degree programme. During the last ten years this same opportunity has been discovered in Africa and India and has worked well in all these contexts and continents. In this talk I shall survey the crucial steps and methods how to establish, and successfully run, international degree programs.

Technical Mathematics and Industrial Mathematics at Johannes Kepler University Linz (JKU)

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The programme in "Technical Mathematics" at JKU started in 1969, which had been modifed several times. From Oct 2003 on it has been following the Bologna scheme (180 ECTS points for the bachelor programme, 120 ECTS points for the continuing master programmes). One of the three master programmes is in "Industrial Mathematics".
From 2005 until 2012 international students from an ERASMUS MUNDUS double degree programme in Industrial Mathematics (together with Eindhoven University of Technology, The Netherlands, and Kaiserslautern University of Technology, Germany) also followed this master programme.
In the presentation we will focus on collaborations with enterprises, suggested master theses and desired resp. actual positions of graduates, both for regular master students as well as for students from the double degree programme.

ECCUM, the creation of a Central Asian MSc with European cooperation

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ECCUM (2015–18) is a project funded by the European Commission, and coordinated by the University of Santiago de Compostela, with the aim of initiating a new postgraduate MSc degree at five universities of Kazakhstan and Uzbekistan. As requested by these universities, the MSc will offer training in mathematical modelling and numerical simulation, and will have a strong connection with industrial stakeholders. The talk will be focused on the origins of the project, its present state, and the planned activities.

Keywords: Erasmus+ Project, Central Asia, postgraduate MSc degree, KA2 - Cooperation for innovation and the exchange of good practices, Capacity Building in Higher Education.

Interdisciplinary approach to the mathematical modelling in a high school – an example from Poland

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Since September 2009 the mathematical modelling experiment is running in a high school near Wroclaw (Poland). Students at that school are from 13 to 16 years old. The project entitled ”Mathematical Modelling as a key to the future - the support of the mathematical education in a grammar-school” is supervised by the ECMI Teaching Center in Wroclaw University of Technology. At the beginning the aim of the venture having the form of pedagogical experiment was understanding by pupils of the role of mathematics in contemporary world. Some modelling structures were copied from the ECMI educational system and applied for a high school rules. The experiment is still unique in Poland and very successful. At the beginning the project was concentrated with selected pupils having the mathematical skills. However three years ago have appeared new challenges. Young students with cross-section hobbies and skills have wished to participate at the modelling activities. For three years that modeling experiment has the form of the STEM style education. It means that for example pupils having interest in biology and mathematics can join group on mathematical modelling related with biological problems. This new style of the running for seven years experiment allows more pupils to understand the role of mathematics at different fields of human activities.

Keywords: high school, mathematical modeling, STEM Education

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Master in Industrial Mathematics (M2i). Learning 4.0 cross-institutional education to solve real problems in industry

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The Master in Industrial Mathematics (M2i) is an official degree jointly delivered by the University of Santiago de Compostela (USC), University of A Coruña (UDC), University of Vigo (UVigo), Carlos III University of Madrid (UC3M) and Technical University of Madrid (UPM) since the current academic year 2013/2014. The M2i duration is 3 semesters and offers two specializations: Modelling and Numerical Simulation. M2i degree promotes a strong dynamic relationship between the main stakeholders: students, Alumni, faculty members and professionals from industry. Teaching staff are professors of Applied Mathematics and related fields with a large experience in the field of numerical simulation and modelling. Some specific topics are delivered by renowned guests from the scientific and industrial fields.

M2i is strongly active in its relations with industry. Due to the Workshop on Industrial Problems we have signed more than 20 agreements with regional, national and international companies that collaborate with M2i. These companies present problems on which the students and teachers work in the Workshops on Industrial Problems and on Modelling. Some of these problems may become the subject of the Master 's dissertation. These companies and technological centers also offer internships to students.

M2i takes advantage of the IT technologies by using a modern videoconferencing system which simultaneously allows students and teachers of the different M2i sites to connect in real time. Additionally, the teaching sessions of a large part of the subjects are recorded so that the students can access the classes from home. Students have also access to professional software during the Master.

Information on jobs offers, courses, seminars is sent regularly to both alumni and current students. Since May 2012 we are very involved in a LinkedIn group for alumni and current master students called "MIM & M2i - Estudiantes y egresados"

In this talk, on behalf of the coordinators of M2i, we highlight the main aspects of the master. Moreover, we will present the first employment survey, and an analysis from the business collaborators in the Workshop on Industrial Problems an also as supervisors of internships.

All information about this Spanish official Master degree can be found at the web site http://m2i.es/en/.

Keywords: Master in Industrial Mathematics, real problems, industry, numerical simulation, modelling.

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The Master degree on applied mathematics to engineering and finance, School of Engineering, Polytechnic of Porto

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The Master on Applied Mathematics to Engineering and Finance of the School of Engineering of the Polytechnic of Porto, Portugal, started its first edition in the scholar year of 2012/13, after being approved by A3ES, the agency for evaluation and accreditation of higher education in Portugal.

This course is divided into four semesters (two scholar years). It emerged in an engineering school with a strong tradition of dialog and collaboration with industry and business partners.

In the second year, the student must conclude his Dissertation/Project/Internship that can be developed in a business or industrial environment, and both students and industrial partners are strongly encouraged to use the internship as the proper way to do it.

We will discuss the benefits and the difficulties of this approach in the point of view of the student, the scientific community and the industrial partner. We will present some success stories on applying this methodology in the above-mentioned master course, showing, at the same time, the benefits that arise from the use of industrial mathematics.

Keywords: Master degree, applied mathematics to engineering, applied mathematics to finance, industrial mathematics, internship in business environment.
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The Master degree of Mathematical Engineering at the University of Porto

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The Master degree of Mathematical Engineering was launched by the Faculty of Sciences, University of Porto, Portugal, in 2003. The course was created following demand by Mathematics students to have a more industry oriented degree that could contribute to their integration in the working market in non-teaching / research activities. The 2-years degree includes a project work for a thesis in the 2nd year, which often is done in external institutions and companies. During the 13 years period of its existence the Master degree evolved, with major changes due to the Bolonha re-structuring of the University degrees within Europe. A considerable number of collaborations between the University and external partners, mostly companies, have been accomplished. The presentation will provide an overview of the Master degree of Mathematical Engineering at the University of Porto, a description of the student experiences in the outside market, as well as perspectives for the future.

Training mathematician in the University of Coimbra: an ECMI master program

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The Master Program in Mathematics in the Department of Mathematics of the University of Coimbra aims to train mathematicians in applied and pure mathematics with a solid mathematical knowledge allowing a future research activity as well as a professional career in life outside the academic world.

The goal of this work is to present the Master Program in Mathematics in the University of Coimbra highlighting its ECMI structure. A review on students success stories will also be presented.

Keywords: Master Program in Mathematics, ECMI program, University of Coimbra.
Acknowledgments. This work was partially supported by the Centre for Mathematics of the University of Coimbra –UID/MAT/00324/2013, funded by the Portuguese Government through FCT/MEC and co-funded by the European Regional Development Fund through the Partnership Agreement PT2020.

MS25: Recrystallization of Si for thin film solar cells: experiments, modelling and numerical simulations

MS25: Recrystallization of Si for thin film solar cells: experiments, modelling and numerical simulations

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Thin-film solar cells exhibit low-cost alternative owing to reduced material and energy consumption in production and are key for the further development of PV applications. A highly promising production process to achieve competitive efficiencies is Liquid Phase Crystallization (LPC). To exploit its full potential, material quality has to be controlled during the production process. This minisymposium presents a series of lectures on the state of the art experimental, mathematical modeling and numerical simulation techniques to control the impact of structural properties such as grain sizes and defects, from the microscopic scale to the large scale continuum description.

Speakers:

Daniel Barragan. Institute for Material Science, TU Darmstadt (Germany). *A Lattice Monte Carlo growth model for silicon including (111) stacking faults and twin boundaries.*

Sibylle Bergmann. Institute of Mathematics, Technical University Berlin (Germany). *Atomistically informed phase-field model for describing solid-liquid interface kinetics in silicon.*

Stefan Gall. Helmholtz Center Berlin for Materials and Energy, Institute for Si-Photovoltaics (Germany). *Polycrystalline silicon films on glass formed by laser-induced liquid phase crystallization.*

Dirk Hauschild. LIMO Lissotschenko Mikrooptik GmbH (Germany). *Interaction of Laser and Semiconductor for Large Area Liquid Phase Crystallization Processes.*

Max Kahnt. Institute for Mathematics, Free University Berlin, (Germany). *Numerical approximations of multi-component multi-phase systems.*

C. Molpeceres. Centro Laser, Universidad Politecnica de Madrid (Spain). *Thermal modelling of laser silicon crystallization.*

Keywords: Liquid Phase Crystalization, thin-Film Solar Cells, Molecular Dynamics Simulation, Phase-Field Modeling, Numerical Methods.

A Lattice Monte Carlo growth model for silicon including (111) stacking faults and twin boundaries

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A Lattice Monte Carlo model for modeling silicon growth which explicitly includes the possibility of (111) stacking faults and twin boundaries is presented. First we show how to construct a suitable lattice model Hamiltonian for this purpose. Second, the model is parametrized for silicon growth using available data on the interface free energies and stacking fault formation energies. Simulations using the model show that the inclusion of stacking faults naturally leads to the emergence of two distinct growth modes of the (111) solid-liquid interface. At an undercooling of 25K, stacking faults do not significantly change the expected growth kinetics at the (111) interface. However, at an undercooling of 50K faulted islands may be sustained, which drastically changes the growth kinetics and the morphology of the growth interface. As the borderlines of stacking fault islands are incommensurate with the matrix crystal, formation of extended defects may be expected via this mechanism. We also calculate interface growth velocities as a function of undercooling and show that multiple twinned silicon crystals may rapidly be grown parallel to the direction of the twin boundaries. Such a crystal growth process is expected to result in crystals with very low density of extended defects. Finally, it is shown that inclusion of stacking faults adds a correction to the location of the (111) interface roughening transition.

Keywords: Lattice Monte-Carlo, silicon growth, solid-liquid interface, interface roughening.
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Atomistically informed phase-field model for describing solid-liquid interface kinetics in silicon

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We propose a phase-field model [2] for describing the liquid-phase crystallization in silicon with atomistically informed expressions for the free energy density, the interfacial energy as well as the temperature and orientation dependent mobility. These expressions are derived systematically from results on the melting point, interface tension [1], free energies [3] and the crystallization velocities directly obtained from molecular dynamics simulations based on the Stillinger-Weber interatomic potential. In contrast to existing phase-field models for Si, our parametrization captures the thermodynamics of the undercooled silicon melt and accounts for the Vogel-Fulcher type behavior of the interface velocities of the solid-liquid interface in the orientations $\{100\}$ and $\{111\}$.

Keywords: silicon, solidification, Stillinger-Weber, Vogel-Fulcher, phase-field model

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Polycrystalline silicon films on glass formed by laser-induced liquid-phase crystallization

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Wafer-based multi- and monocrystalline silicon solar cells with a silicon thickness of about 180μm are currently dominating the photovoltaic market. The reduction of the silicon thickness is an appealing way to further bring down costs because even very thin crystalline silicon solar cells feature the potential for very high efficiencies. However, the preparation and subsequent processing of very thin silicon wafers poses a big challenge.

The formation of high-quality silicon thin-films formed directly on large-area low-cost glass substrates represents a very attractive alternative to the well-established wafer technology. So far, the most promising technique to prepare crystalline silicon thin-films on glass is based on liquid-phase crystallization of silicon using either a line-shaped electron beam or a line-shaped laser beam. The resulting polycrystalline silicon films with a thickness of about 10μm feature a material quality comparable to multicrystalline silicon wafers.

The presentation will give an overview on the current status of the formation of polycrystalline silicon films on glass using a line-shaped laser beam. Among other things the contribution will address the influence of the crystallization parameters (scan velocity, temperature) as well as the crystallization configuration (with and without seed) on the properties of the polycrystalline silicon films, especially with regard to the crystallographic structure of the films.

Keywords: liquid-phase crystallization, thin-film, silicon, polycrystalline

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Interaction of laser and semiconductor for large area liquid phase crystallization processes

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The use of laser photons for selective dynamic heating of thin films and surfaces can be used to activate and improve specific material properties and to generate new material structures and compositions with application specific functionalities. We will introduce a technology that enables the individual forming of laser beam profiles to enable large area surface heat treatment. The defined selection of laser beam parameter like intensity, power and beam shape in combination with an adjustable dwell time open a six magnitude large field of numeric controlled processing energy that can be used for precise heating and melting of e.g. a-Si layer on glass. Due to the dynamic heating with the process optimized laser beam profile the transformation into polysilicon can be achieved without destroying the substrate material. We will show examples of scaling the laser crystallization source to a multi square meter per minute productivity for next generation high performing PV products.

Keywords: Laser, beam shaping, micro-optics, liquid phase crystallization, polysilicon.

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Numerical approximations of multi-component multi-phase systems

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We consider a non-isothermal multi-component multi-phase field model. We subsequently discretize implicitly in time and with linear finite elements. The arising algebraic problem is formulated in two vector-valued variables. One represents the order parameters, i.e. the multi-phase field as well as the chemical components, and the other captures the thermodynamic (temperature and chemical) potentials. The inheritance of the thermodynamical consistency to the discrete model is investigated. We solve this saddle point problem numerically by a non-smooth Schur–Newton approach using truncated non-smooth Newton multigrid methods. Adaptive mesh refinement is performed in each time step using a hierarchical error estimator. An application in Silicon liquid phase crystallization is considered.

Keywords: multi-component, multi-phase, thermodynamic consistency, adaptive, finite elements, non-smooth, saddle point problem, multigrid
Acknowledgments. The work was supported by the Helmholtz Virtual Institute HVI-520 “Microstructure Control for Thin-Film Solar Cells”.

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Thermal modelling of laser silicon crystallization

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Laser crystallization has been widely applied to formation of polycrystalline silicon films and has been introduced to fabrication process of polycrystalline silicon thin film transistors (poly-Si TFTs) and solar cell applications. In the latter case, the crystallization of amorphous silicon (a-Si) thin films is one of the most promising methods for diminishing costs and improving solar cells efficiency.

During the laser crystallization, controlled mainly by the irradiation time and the material absorption depth for the wavelength used, the incident energy of the laser is partially absorbed by the a-Si film, heating it. When the material is melted or heated for a time long enough to a temperature close to the melting point, crystallization of a-Si is obtained. But if the vaporization temperature is reached, ablation effects are expected and the annealing process becomes ineffective.

In this work we present a study of the irradiating time and wavelength influence in laser annealing of amorphous silicon thin films, using both continuous wave and pulsed laser sources emitting at wavelengths ranging from UV to IR. Experimental characterization of the crystallized samples have been obtained by MicroRaman spectroscopy. A simple thermal finite element model (FEM) has been developed in COMSOL Multiphysics to simulate the process by solving numerically the two dimensional non-linear heat transfer equation with a steady heat source. The local temperature evolution in the irradiated area given by the FEM model is compared to the crystalline fraction profiles. The numerical model developed helps to understand the physics underlying and determine the process parameters in which crystalline silicon is obtained without damage or ablation of the silicon surface.

Keywords: Amorphous silicon, Laser crystallization, Simulation, COMSOL Multiphysics.
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MS26: Stochastic inverse problems

MS26: Stochastic inverse problems

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Stochastic inverse problems have received an increasing amount of attention in recent years, especially in the context of physical phenomena that can be described by partial differential equations (PDEs). Real-world applications often require the consideration of different sources of uncertainty (in boundary conditions, coefficients etc.) in the PDE model. Stochastic inverse problems seek to infer the parameters characterizing the physical model from indirect measurements in the presence of multiple sources of uncertainty. The aim of this minisymposium is to present recent work on theoretical and numerical aspects for stochastic inverse problems involving partial differential equations. The main focus lies on Bayesian inverse problems arising in subsurface flow simulations, structural mechanics and other engineering applications.

Stochastic inverse problems are of a very high importance for engineering applications. The application problems addressed in this minisymposium can be of interest for wider circle of experts from various fields of industrial mathematics such as structural mechanics, environmental simulations, medical and subsurface imaging.

Speakers

Matthew Dunlop. University of Warwick (England). *Hierarchical Bayesian Level Set Inversion.*

Björn Sprungk. Chemnitz University of Technology (Germany). *Bayesian Inverse Problems and Kalman Filter.*

Tom Lahmer. Bauhaus University of Weimar (Germany). *Assessment of Uncertainties in the Results of Inverse Source Problems with Applications to Steel.*

Nataliya Togobytska. Weierstrass Institute, Berlin (Germany). *Uncertainty quantification in environmental simulations.*

There is no direct industrial participation in this minisymposium, however a work that will be presented by Nataliya Togobytska is a joint work with industrial partners (DHI-WASY GmbH, Berlin).

Keywords: Uncertainty quantification, Bayesian inverse problems, Bayesian level set inversion, Kalman filter

Hierarchical Bayesian level set inversion

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The level set approach has proven widely successful in the study of inverse problems for interfaces, since its systematic development in the 1990s. Recently it has been employed in the context of Bayesian inversion, allowing for the quantification of uncertainty within the reconstruction of interfaces. However the Bayesian approach is very sensitive to the length and amplitude scales in the prior probabilistic model. This paper demonstrates how the scale-sensitivity can be circumvented by means of a hierarchical approach, using a single scalar parameter. Together with careful consideration of the development of algorithms which encode probability measure equivalences as the hierarchical parameter is varied, this leads to well-defined Gibbs based MCMC methods found by alternating Metropolis-Hastings updates of the level set function and the hierarchical parameter. These methods demonstrably outperform non-hierarchical Bayesian level set methods.

Keywords: Inverse problems for interfaces, Level set inversion, Hierarchical Bayesian methods.
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Bayesian inverse problems and Kalman filter methods

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In recent years the interest and research activity in uncertainty quantification (UQ) for complex systems modelled by partial differential equations (PDEs) has increased significantly. Beside the *forward problem* where a given probability law for the uncertain input data is propagated to the corresponding law of the solution of the PDE, the *inverse problem* has received more and more attention in the UQ community.

Within UQ the inverse problem consists of incorporating available noisy observational data of the solution of the PDE into the prior probability law of the uncertain input. Mathematically this can be done by conditioning the prior probability measure on the observations and results in a conditional or posterior measure for the input. The posterior is given by Bayes' rule up to a normalizing constant and the computational challenge is to sample or integrate w.r.t. it.

Since Bayesian inverse problems have gained much attention in the scientific computing community in the last few years, numerous algorithms and numerical methods have been proposed for their solution. We provide a short introduction to Bayesian inverse problems and focus on Kalman Filter methods, in particular, the *Ensemble Kalman Filter* (EnKF) [3] and the *Polynomial Chaos Kalman Filter* (PCKF) [4, 5], which have been recently proposed for UQ in association with inverse problems. We analyze the EnKF and PCKF applied to nonlinear stationary Bayesian inverse problems. In a sequential data assimilation setting, such stationary problems arise in each step of either filter. We give a new interpretation of the approximations produced by these two popular filters in the Bayesian context and prove that, in the limit of large ensemble or high polynomial degree, both methods yield approximations which converge to a well-defined random variable termed the analysis random variable. We then show that this analysis variable is more closely related to a specific linear Bayes estimator than to the solution of the associated Bayesian inverse problem given by the posterior measure. This suggests limited or at least guarded use of these generalized Kalman filter methods for the purpose of uncertainty quantification.

Keywords: Uncertainty quantification, Bayesian inverse problems, Kalman filter, polynomial chaos
Acknowledgments. All authors were supported by the DFG priority program 1324.

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Assessment of uncertainties in the results of inverse source problems with application in steel engineering

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We discuss computational aspects of the inverse and ill-posed problem of identifying residual stresses in steel structures which corresponds to an inverse source problem in linear elasticity. The studies aim in optimizing experimental setups and in quantifying uncertainties in the results of an inverse computation. Residual stresses are critical, e.g., in steel structures which have been loaded thermally in the construction process. The residual stresses may lead to undesired deformations or even to concerns w.r.t the stability of the structures. An identification of the stress fields by inverse analysis is a prerequisite to successfully remove the stresses by thermal treatment. The presented approach is destruction-free and considers moderate thermal loadings. Due to these loadings deformations occur which can be recorded by high resolution laser scanners. The latter serve as input for the identification problem, where residual stresses are to be recovered from measured displacements. As the inverse problem is ill-posed, it requires regularization, where the minimal error method, a variant of the Landweber method, is applied together with a discrepancy principle.

After an identification, the quality of the identified stress fields depend on a list of parameters, e.g., the number of heat excitations, smoothing of the data, the noise in the measurements, the error assumed for the definition of stopping criteria, and further uncertainties in other model parameters, like the stiffness or the thermal conductivity and thermal expansion coefficient of the structure.

The influence of these factors in the quality of the identified stress fields will be analyzed and effects of randomness in the solutions of the inverse problems quantifies by means of Sobol Indices.

Keywords: Residual Stress Identification, Inverse Problems, Uncertainty Quantification

Uncertainty quantification in environmental simulations

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Uncertainty is a structural and inevitable characteristic of all hydrological processes arising from the essential complexity of the related natural systems. The quantification of uncertainty in the geologic properties of the subsurface is of major interest in subsurface flow applications, and necessary to account for the risk within planning and decision-making.

We consider the inverse problem of identifying the permeability of the subsurface from hydraulic head measurements based on the steady Darcy model of groundwater flow. For the identification of unknown geometric and physical parameters in the model we adopt a Bayesian framework. This approach provides a quantification of the uncertainty via the posterior distribution of unknown parameters given noisy data and prior distribution of parameters. For numerical experiments, we compare two different computational approaches to explore the posterior, namely Markov Chain Monte Carlo and Kalman filter methods. These numerical algorithms provide estimates of the permeability and the uncertainty associated with it, and only require forward model evaluations.

Keywords: Bayesian inverse problems, Markov Chain Monte Carlo, Kalman filter, subsurface flow.
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MS27: 10 years of Portuguese Study Groups with industry

MS27: 10 years of Portuguese Study Groups with Industry

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This mini-symposium provides an overview of the implementation and evolution of European Study Groups (ESGI) in Portugal, describing our experience and some industrial problems dealt with, the challenges that had to be overcome and examples of successful and less successful stories.

Skeakers:

J. Orestes Cerdeira. Dep. de Matemática and Centro de Matemática e Aplicações, Faculdade de Ciências e Tecnologia da Universidade Nova de Lisboa, Portugal. *Warehouse storing and collecting of parts: a challenge addressed on the* 65^{th} *European Study Group with Industry.*

Eliana Costa e Silva. CIICESI, ESTGF, Polytechnic Institute of Porto, Portugal. *Scheduling aircraft engines repair process: a challenge addressed on the* 86^{th} *European Study Group with Industry.*

A. Ismael F. Vaz. Department of Production and Systems, School of Engineering, University of Minho, Portugal. *A scheduling application to a molding injection machine: a challenge addressed on the* $109th$ *European Study Group with Industry.*

Ana Moura. LEMA/CMUP, Neoturf, Portugal. *A routing/assignment problem in garden maintenance services: a challenge addressed on the* 86^{th} *European Study Group with Industry.*

Adérito Araújo. CMUC, Department of Mathematics, University of Coimbra, Portugal. *A characterisation of ESGIs problems.*

The first talk, presented by Jorge Orestes Cerdeira, describes a problem submitted by Grohe, a sanitary fittings manufacturer. The original problem, presented at the 65^{th} ESGI, stated that the company would like to reduce the costs resulting from storing and collecting items in the warehouse. Storage and collecting operations are accomplished by forklifts that operate inside the corridors. In this talk, it is shown how to convert the problem of determining optimal corridor tasks into an assignment problem [3], as well as that the problem of assigning forklifts to corridors and settling how each forklift should visit the corridors assigned to it can be formulated as a capacitated vehicle routing problem [4].

The second talk addresses a real world scheduling problem, presented at the 86^{th} ESGI, concerning the repair process of aircraft engines by TAP - Maintenance $\&$ Engineering (TAP-ME), which is the maintenance, repair and overhaul organization of TAP Portugal, Portugal's leading airline. The company's Engine Shop Production Planning Department aimed to have a mathematical model for the engines repair process that would determine the optimal sequencing of tasks within the workstations, in order to minimize total weighted tardiness, while assigning relative priorities to different clients. Because of its similarities with the classical jobshop problem [1] the team, here represented by Eliana Costa e Silva, developed a mixed integer programming model for the specific issues of the TAP engine repair process. Computational experiment on a real instance provided by TAP-ME from a regular working week was successful in finding an optimal solution. Results of the model using benchmarking instances available in the literature [2] will also be presented.

In the last talk of the first day, Ismael Vaz presents in detail the challenge of optimizing the scheduling of a shoes injection moulding machine. The solution proposed for this problem at the $109th$ ESGI, modeled it as an integer mathematical optimization problem [5, 6]. The model was coded in AMPL [7], allowing state-of-the-art integer programming solvers to be used and tested. The Gurobi [8] solver,

available through the NEOS [9] server platform, was used to provide a solution for a particular shoes manufacturing order. The numerical results for two types of optimization problems by considering different sets of constraints are discussed.

The second session of the *10 years of Portuguese Study Groups with Industry* mini-symposium starts with a talk given by a mathematician (Ana Moura). They will address the problem posed by Neoturf to the 2012 Portuguese ESGI from both the academic and industrial perspectives. The aim of this challenge was to define a procedure for scheduling and routing efficiently its clients of garden maintenance services, over a wide geographic region. The total distance travelled then weighs heavily on the company costs and the original statement of the problem focused on a reduction of these costs, while satisfying agreements with its clients. On this talk the authors present a mixed integer linear programming formulation for the problem [10], discuss the limitations on the size of instances that can be solved to guarantee optimality, present a modification of the Clarke and Wright [11] heuristic for the vehicle routing with time windows [12, 13], and report some results obtained with Neoturf data.

This mini-symposium ends with a talk presented by Adérito Araújo, overviewing the first ten years of European Study Groups in Portugal, focusing on what the authors believe to be the main issues arising in this and similar initiatives. After a brief description of the very beginnings of Portuguese ESGIs, which they hope to be of interest for anyone deciding to embark on such an enterprise, the different types of problems posed by industry in the Portuguese series will be discussed. Finally, a characterisation of what the authors perceive as the main problems arising in the relationship between the industrial and the academic communities in Portugal is presented. In spite of specific idiosyncrasies, we believe that there is much to be learnt from sharing these and similar experiences, and hope that this will be of interest to ESGI organisers in other countries.

Keywords: Portuguese Study Groups, ESGIs, Industrial Mathematics, Aeronautics, Footwear Industry.

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Warehouse storing and collecting of parts: a challenge addressed on the 65th European Study Group with Industry

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Warehouse operation planning is a sensible matter given the large contribution of this sector to the total costs of many companies. This justifies the intense work dedicated to this subject. We refer to [2] for an extensive review of the topic, linking views from academic researchers and warehouse practitioners.

Manufacturers and suppliers are interested in reducing the costs resulting from storing and collecting items in the the warehouse. Storage and collecting operations are accomplished by forklifts that operate inside the corridors. Each forklift cannot carry more than one item in each course. Hence, a course consists of:

(a) collecting an item from a depot located near the entrance of the corridor, carrying it to a store position i, move to some store position j to pick another item, and take it to the depot; or
(b) carry an item from the depot to a store position i, and come back to the depot; or
(c) leaving the depot unloaded to collect an item at storage location j and return to the depot.

If the storage locations i and j are not on the same side of the corridor, the courses of type (a) require some extra work. Indeed, once inside the corridor, the forklift can only work on one side. To operate on the opposite side requires that the orientation of the forks has been previously reversed, which has to be done outside the corridor.

The greatest concern is to reduce the high costs due to the wear and tear of the forklifts. This is directly proportional to their usage and is mostly determined by the distances covered on the storage/collection operations. Costs can be significantly reduced if the corridor tasks are carefully settled. Additionally, it is of concern to find an efficient way to define which forklift should operate on each corridor, and the order by which the forklifts should visit the corridors.

We give to both problems formulations that fit in the framework of combinatorial optimization. Specifically, we show how to convert the problem of determining optimal corridor tasks into an assignment problem [1], and show that the problem of assigning forklifts to corridors and settling how each forklift should visit the corridors assigned to it can be formulated as a capacitated vehicle routing problem [3].

Keywords: Assignment problem, traveling salesman problem, capacitated vehicle routing.
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Scheduling aircraft engines repair process: a challenge addressed on the 86^{th} European Study Group with Industry

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In this talk we address a real world scheduling problem concerning the repair process of aircraft engines by TAP - Maintenance & Engineering (TAP-ME), which is the maintenance, repair and overhaul organization of TAP Portugal, Portugal's leading airline.

In May 2012, TAP-ME participated in the 86^{th} European Study Group with Industry to consult with academics to find ways to optimize and reduce their engines repair turn around time. The company's Engine Shop Production Planning Department aimed to have a mathematical model for the engines repair process that would determine the optimal sequencing of tasks within the workstations, in order to minimize total weighted tardiness, while assigning relative priorities to different clients.

Because of its similarities with the classical jobshop problem [5], we developed a mixed integer programming model for the specific issues of the TAP engine repair process. The formulation is based on the flexible job shop scheduling [2, 3] and allows the repair operations of the engines to be executed on the same workstation by any processor of a given set [1]. We use binary variables to assign operations to processors and to describe the precedences between pairs of operations that are performed in the same processor, along with the corresponding linear ordering constraints [6]. We use continuous variables to define the starting times of each part repair operation and the tardiness of each engine.

Computational experiment on a real instance provided by TAP-ME from a regular working week was successful in finding an optimal solution. We also report results of the model using benchmarking instances available in literature [4].

Keywords: Real world scheduling; Flexible job shop; Mixed integer linear programming; Engine repair process; European Study Group with Industry; ESGI; Industrial Mathematics.
Acknowledgments. The third author was partially supported by the Portuguese Foundation for Science and Technology (FCT-Fundação para a Ciência e a Tecnologia), through CMA - Center of Mathematics and Applications, Project UID/MAT/00297/2013.

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A scheduling application to a molding injection machine: a challenge addressed on the 109th European Study Group with Industry

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The 109th European Study Group with Industry (ESGI) took place from May 11th to May 15th, 2015, at the Department of Production and Systems of the School of Engineering, University of Minho. Industries are requested to pose mathematical challenges to a set of experienced mathematical researchers, which dedicate a full working week in providing a solution, or avenues to get a solution, to the posed challenges. Six mathematical challenges where submitted by local companies with a national and international impact, operating in the Portuguese market and overseas.

The posed challenges were: *Modelling and optimization of production scheduling*, where a textile company posed the challenge to model the full production operations; *Physical model of MDF boards*, where the challenge to provide a physical model of MDF boards was proposed; *Setting the Reserve Fleet*, where a public transportation company challenged the group to provide an optimal vehicles reserve fleet; *Surgical cases packages*, where an optimal set of surgical cases packages for use in surgical wards was to be obtained; *Prediction model to textile parameters*, where the combination of yarns and yarns types were to be obtained in order to get a textile with given properties; and *Optimization of a shoes injection moulding machine*, where the scheduling of an injection moulding machine was addressed. A detailed report with the group achievements was delivered to the corresponding companies, where a solution for the challenge and/or avenues for future collaborations where proposed.

In this talk we describe in detail the challenge of optimizing a shoes injection moulding machine. The mathematical problem was modeled as an integer mathematical optimization problem [1, 2]. The model was coded in AMPL [3], allowing state-of-the-art integer programming solvers to be used and tested. The Gurobi [4] solver, available through the NEOS [5] server platform, was used to provide a solution for a particular shoes manufacturing order. We discuss numerical results for two types of optimization problems by considering different sets of constraints.

Keywords: Injection moulding machine, scheduling, integer programming, European Study Group with Industry.
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A routing/assignment problem in garden maintenance services: a challenge addressed on the 86^{th} European Study Group with Industry

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We address a routing/assignment problem posed by Neoturf, which is a Portuguese company working in the area of project, building and garden's maintenance. The aim is to define a procedure for scheduling and routing efficiently its clients of garden maintenance services. The company has two teams available throughout the year to handle all the maintenance jobs. Each team consists of two or three employees with a fully-equipped vehicle capable of carrying out every kind of maintenance service. At the beginning of each year, the number and frequency of maintenance interventions to conduct during the year, for each client, are agreed. Time windows are established so that visits to the client should occur only within these periods. There are clients that are supposed to be always served by the same team, but other clients can be served indifferently by any of the two teams. Since clients are geographically spread over a wide region, the total distance traveled while visiting clients is a factor that weighs heavily on the company costs. Neoturf is concerned with reducing these costs, while satisfying agreements with its clients. We give a mixed integer linear programming formulation for the problem [1], discuss limitations on the size of instances that can be solved to guarantee optimality, present a modification of the Clarke and Wright [2] heuristic for the vehicle routing with time windows [4, 3], and report preliminary computational results obtained with Neoturf data.

The problem addressed in this paper was presented by Neoturf at the 86^{th} European Study Group with Industry, held at ISEP/IPP, School of Engineering, Polytechnic of Porto, 7 - 11 May 2012.

Keywords: operational research; scheduling; vehicle routing with time windows; integer programming; European Study Group with Industry.
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A characterisation of ESGIs problems

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In this talk we shall provide an overview of the first ten years of European Study Groups in Portugal, focusing on what we believe to be the main issues arising in this and similar initiatives.

We shall first give a brief description of the very beginnings of Portuguese ESGIs, which we hope may be of interest for anyone deciding to embark on such an enterprise. We will then discuss the different types of problems that are posed by industry in the Portuguese series, touching only briefly on specific examples, as these will be mainly addressed in separate talks. Finally, we shall characterise what we perceive as the main problems arising in the relationships between the industrial and the academic communities in Portugal.

In spite of their own idiosyncrasies, we believe that several things may be learnt here which are of interest to organisers of ESGIs in other countries and we shall address this in the last part of the presentation.
Keywords: European Study Groups with Industry.

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MS28: Finite volume schemes for degenerate problems

MS28: Finite Volume schemes for degenerate problems

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This minisymposium is a response to the growing use of finite volume schemes combined with finite element schemes in degenerate problems and is intended to bring together developers and researchers from academia and industry. Degenerate problem arises from multifluid flow in porous media or in medicine model as the breast cancer or bone healing model.
Saturations of oil, gas and water, or densities of cells are positive quantities, hence it is crucial to propose numerical schemes ensuring the physical properties as the positiveness and conservation. The goal of this minisymposium is to shed light on recent advances, for instance, in nonlinear control volume finite element scheme or nonlinear monotone scheme for degenerate problems with anisotropic and heterogeneous diffusion tensor over general meshes.

Speakers:

Cindy Guichard. Université Pierre et Marie Curie, Paris (France). *A degenerate coupled parabolic problem arising in the study of the root-nutrient system.*

Moustafa Ibrahim. Ecole Centrale de Nantes (France). *Nonlinear CVFE scheme for simulating a breast cancer model.*

Mladen Jurak. University of Zagreb (Croatia). *On Double Porosity Model for Two-Phase Flow in Porous Media.*

Mazen Saad. Ecole Centrale Nantes (France). *Numerical analysis for partially miscible two-phase two component flows in porous media.*

A degenerate coupled parabolic problem arising in the study of the root-nutrient system

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We consider a simplified model for the root-nutrient system inspired by [1, 4]. Hence we consider here the solution h, c of the following system of equations:

$$\partial_t \Theta(h) - \mathrm{div}(K\nabla h) = f, \tag{1}$$

$$\partial_t(\Theta(h)c + \varphi(c)) - \mathrm{div}(cK\nabla h + A\nabla c) = g. \tag{2}$$

In the above equations, h denotes the hydraulic head, $\Theta(h)$ is the capacity function, K is the permeability of the porous medium ((1) is then a simplified form of the Richards equation). We denote by c the concentration of the nutrient in the water phase, by $\varphi(c)$ the amount of nutrient per unit volume which is adsorbed by the porous medium. Then A stands for a diffusion operator, including the effects of dispersion in porous media.

System (1)-(2) is approximated, following the gradient schemes framework [3, 2]. This framework allows to develop convergence proofs which simultaneously encompass a variety of numerical schemes as for instance conforming finite elements with mass lumping, mixed finite elements and mimetic finite differences. The scheme for approximating (1) is a simple discrete translation of the continuous equation, which allows for deriving some estimates on the discrete solution denoted $h_{\mathcal{D}}$. The discrete field such obtained is then used in the discretization of (2), leading to additional estimations. Unfortunately, it is not possible to write the scheme by a simple discrete translation of the continuous equation. In fact, the discrete unknown is not c, but it is $\varphi(c)$; this choice ensures that the nonlinear equations to solve are differentiable with respect to the discrete unknowns, and therefore the Newton-Raphson method may be used without singular matrices. We will focus on the techniques used in order to prove the convergence to a weak solution of the continuous equations.

Keywords: gradient schemes, root-nutrient system, degenerate parabolic equations.

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Nonlinear CVFE scheme for simulating a breast cancer model

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Breast cancer is not just a disease, but rather a complicated interaction of many abnormal features and many different cell types, which are situated in a heterogeneous environment of normal tissue. A significant challenge on the mathematical modeling of breast cancer growth arises due to the interactions of breast cancer with a complicated and structured microenvironment of healthy tissue.

Many of the spatial models [1, 2, 3] in breast cancer modeling are based on nonlinear partial differential equations (PDEs) that include spatial heterogeneity and orientational tissue structure. For instance, Enderling and al. propose a mathematical model of breast cancer development and its progression.
In this model, there is a description of how the growing solid tumor invades and interacts with its surrounding environment in terms of partial differential equations. Since, we assume that mutations at specific genes are necessary for the initiation or early progression of breast cancer development; the model firstly shows the stepwise mutations from a normal breast stem cell to a tumor cell, secondly it shows that these mutations will formed a field of cells with theses mutations through clonal formation of the breast, and finally the tumor will arise from within this area.

Our motivation is a finite volume scheme similar to that proposed in [5] and for a modified model proposed in [3]. First, we show that the numerical scheme preserves the essentiel physical properties of the model such as the discrete maximum principle and the boundedness of the discrete solution (*a priori* estimates). Next, by the use of a compactness criterion [4], we establish the convergence of the discrete solution towards a weak solution of the continuous model. Finally, we present multiple numerical simulations to show the efficacy of the scheme to capture the breast cancer development.

Keywords: Mathematical model, Breast cancer, cancer development, mutation, finite volume method.

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On double porosity model for two-phase flow in porous media

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We consider modeling of fractured porous media by homogenization theory. Incompressible two-phase flow is considered in a periodic porous medium with thin fissures. Completely homogenized double porosity model is obtained by letting matrix-block size tend to zero, linearizing the *imbibition equation* and then letting relative width of the fissures to zero.

We discuss different ways of linearizing the imbibition equation which lead to different simplified double porosity models. These models are then compared numerically with the aim to improve precision of simplified double porosity model for the two-phase flow. Finite volume method is designed for efficient simulation of considered double porosity models and numerical simulations are presented showing relevance and complexity of different models.

Keywords: two-phase flow, double porosity model, finite volume method.
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Numerical analysis for partially miscible two-phase two component flows in porous media

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We propose and analyze the convergence of a combined finite volume–nonconforming finite element scheme on general meshes for a partially miscible two-phase flow model in anisotropic porous media. We consider herein a porous medium saturated with a fluid composed of two phases (liquid and gas) and a mixture of two components. The first component is considered to be an aqua component and it is supposed to be only present in the liquid phase (no vapor of water due to evaporation). The second component is considered to be a constituent which can be present is the two phases such as hydrogen or CO2. We investigate the modelling compositional two-phase flow with focus on hydrogen appearance in nuclear waste industry [1] and perspectives on underground CO2 sequestration [3]. This model includes capillary effects and exchange between the phases. The diffusion term, which can be anisotropic and heterogeneous, is discretized by piecewise linear nonconforming triangular finite elements. The other terms are discretized by means of a cell-centered finite volume scheme on a dual mesh. The mobility of each phase is decentered according to the sign of the velocity at the dual interface. Next, a priori estimates on the velocities and a function of the saturation that denotes capillary terms are established. The convergence of the scheme is proved thanks to estimates on the two pressures which allow to show estimates on the discrete time and compactness results in the case of degenerate relative permeabilities. A major point in the construction of the combined scheme is to use particular averaging formula for the dissolution function arising in the diffusion term [5, 4, 6, 2]. We show also a simulation of hydrogen production in nuclear waste management.

Keywords: partially miscible, porous media, degenerate compressible, finite volume method.

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MS29: Differential equation models of propagation processes

MS29: Differential equation models of propagation processes

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The aim of this mini symposium is to present results about modeling different propagation processes by using ODEs and PDEs. Epidemic propagation on networks is considered with focusing on the relation between the structure of the network and the qualitative behavior of the solutions of the corresponding differential equations. Old and new product formulas for evolution equations will be surveyed. Applications to numerical analysis and operator theoretic properties of the evolution equation will also be given.

Speakers:

Diana Knipl, Department of Mathematics, University College London (UK).*Rich dynamics in simple disease spread models on travel networks.*

Gergely Röst, Institute of Mathematics, University of Szeged (Hungary).*Impact of non-Markovian recovery on network epidemics.*

Joan Saldaña, Universitat de Girona (Spain).*Density-dependent diffusion rates and the initial phase of epidemics on heterogeneous metapopulations.*

András Bátkai, Bergische Universität Wuppertal (Germany). *Product formulas for non-autonomous evolution equations.*

Peter L. Simon, Institute of Mathematics, Eötvös Loránd University, Budapest Hungary.*Approximating epidemic propagation on networks by low-dimensional ODEs.*

Rich dynamics in simple disease spread models on travel networks

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Recent epidemics like the 2002–2003 SARS outbreak, the 2009 influenza pandemic, and the 2014 Ebola crisis illustrated that an infectious agent can spread across the globe very rapidly via transportation networks. We show that incorporating spatial dispersal of individuals into a simple vaccination epidemic model may give rise to a model that exhibits rich dynamical behaviour, not normally seen in simple epidemic models. Our model is suitable to describe the spread of an infectious disease when individuals are traveling between distinct locations, such as major cities. In disease transmission models, the usual situation is that the underlying differential system has a "disease-free" steady state and a single "endemic" equilibrium (the disease is maintained in the population without the need for external inputs). In contrast, we find that up to nine equilibria can exist in our model. Stability of steady states, their bifurcations, and the global dynamics are investigated with analytical tools, numerical simulations, and rigorous set-oriented numerical computations. Investigating the long time behaviour of solutions in epidemic models provides key knowledge for determining the final epidemic outcome and identifying adequate intervention measures. A rich equilibria structure implies that the disease dynamics is sensitive to the model parameters and initial conditions. It also allows a variety of different final epidemic outcomes, which makes disease control and mitigation challenging.

Keywords: vaccination epidemic model, spatial spread, patch model, bifurcation analysis, rigorous numerics.

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Impact of non-Markovian recovery on network epidemics

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We present a generalization of pairwise models to non-Markovian epidemics on networks. For the case of infectious periods of fixed length, the resulting pairwise model is a system of delay differential equations (DDEs), which shows excellent agreement with results based on explicit stochastic simulations of non-Markovian epidemics on networks. Furthermore, we analytically compute a new R_0-like threshold quantity and an implicit analytical relation between this and the final epidemic size. In addition we show that the pairwise model and the analytic calculations can be generalized in terms of integro-differential equations to any distribution of the infectious period, and we illustrate this by presenting a closed form expression for the final epidemic size. By showing the rigorous mathematical link between non-Markovian network epidemics and pairwise DDEs, we provide the framework for a deeper and more rigorous understanding of the impact of non-Markovian dynamics with explicit results for final epidemic size and threshold quantities.

We study in details some typical families of distributions (such as gamma, uniform and lognormal), showing that higher variance in the recovery times generates lower reproduction numbers and different epidemic curves within each distribution family. We also show that knowing the expected value and the variance of the recovery times is not sufficient to determine the key characteristics of the epidemics such as initial growth rate, peak size, peak time and final epidemic size. For accurate predictions, more detailed information on the distribution of the infectious period is required, thus carefully estimating this distribution in the case of real epidemics has paramount public health importance.

Keywords: network epidemics, non-Markovian epidemics, pairwise model, delay differential equation

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Density-dependent diffusion rates and the initial phase of epidemics on heterogenous metapopulations

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One way to model the spread of epidemics on spatially distributed populations is based on the metapopulation approach. A metapopulation consists of a set of local populations living in patches which are connected to each other by migratory flows. In the simplest models, patches are labeled by their connectivity (or degree) whereas their spatial location within the metapopulation is neglected. Moreover, migratory flows among patches occur at random and with constant diffusion rates [1, 3, 4].

In this talk, following the continuous-time formulation introduced in [3], we present an extension of these models where diffusion rates depend on the population at departure patch (nonlinear density-dependent diffusion rates). A positive density dependence reflects the fact that high population densities increase competition effects among their individuals and induce emigration from heavily populated locations. On the contrary, a negative density dependence corresponds to conspecific attraction, i.e., the tendency for individuals of a species to settle near conspecifics.

We will analyse the impact of such migration patterns on the epidemic outbreaks occurring within a metapopulation. In particular, we will see that, depending on the exponent α of the nonlinear diffusion rate which is assumed to be of the form $D(\rho_i) = D_0 \cdot (\rho_i/\rho^0)^\alpha$ with ρ_i denoting the size of i-population and ρ^0 the mean population per patch, epidemic outbreaks do not always occur in the most populated areas as one might expect. In addition to such a study of the early stage of epidemics, population profiles arising from different diffusion rates are also considered, as well as how the whole population is distributed among heavily and lightly populated patches in metapopulations whose architecture is described by scale-free networks.

Keywords: Epidemics, metapopulations, non-linear diffusion.
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Product formulas for nonautonomous evolution equations

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Old and new product formulas for evolution equations will be surveyed. Applications to numerical analysis and operator theoretic properties of the evolution equation will be also given. The main result can be formulated in the following way. Suppose that:

- The domain $D := D(A(t))$ is dense in X and is independent of $t \in \mathbb{R}$.
- For each $t \in \mathbb{R}$ the operator $A(t)$ is the generator of an analytic semigroup $\mathrm{e}^{\cdot A(t)}$. For all $t \in \mathbb{R}$, the resolvent $R(\lambda, A(t))$ exists for all $\lambda \in \mathbb{C}$ with $\Re\lambda \geq 0$ and there is a constant $M \geq 1$ such that
$$\|R(\lambda, A(t))\| \leq \frac{M}{|\lambda| + 1}$$
for $\Re\,\lambda \geq 0$, $t \in \mathbb{R}$. The semigroups $\mathrm{e}^{\cdot A(t)}$ satisfy $\|\mathrm{e}^{sA(t)}\| \leq M\mathrm{e}^{\omega s}$ for absolute constants $\omega < 0$ and $M \geq 1$.
- There exist constants $L \geq 0$, $\alpha \geq 0$ and $0 < \gamma \leq 1$, such that
$$\|(A(t) - A(s))A(0)^{-\alpha}\| \leq L|t - s|^{\gamma} \text{ for all } t, s \in \mathbb{R}.$$

Then we can formulate the following result:
Suppose that that there is $\beta \in (0, 1]$ with $\gamma - \eta - \beta > 0$ such that $(-A)^{-\beta} \in \mathcal{A}(X)$. Then $U(t, s) \in \mathcal{A}(X)$ for $t > s$. Further, there is $C > 0$ such that

$$\left\| U(t,s) - \prod_{k=0}^{n-1} \mathrm{e}^{\frac{t-s}{n} A(s+k\frac{t-s}{n})} \right\|_{\mathcal{A}} \leq \frac{C}{n^{\gamma-\eta-\beta}}$$

holds.

Keywords: operator ideals, nonautonomous equations, evolution families.
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Approximating epidemic propagation on networks by low-dimensional ODEs

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The pairwise ODE model for SIS (susceptible-infected-susceptible) epidemic propagation was developed for regular random networks (where each node has the same degree). This model is formulated in terms of the number of infected nodes and the number of SI and SS edges. For heterogeneous networks (with a given degree distribution) the heterogeneous pairwise model was introduced, however, the size of this system is of order K^2, where K is the number of different degrees in the network. Thus for random graphs with long tail degree distribution (such as power-law random graphs) this system is too large for numerical investigation. An approximating system of size order K, called compact pairwise model, was developed to overcome this difficulty. Recently, an even simpler approximating model, containing only four differential equations, has been developed by the author and co-workers [1]. This system is based on a new closure relation incorporating the second and third moment of the degree distribution. A summary about these models is shown and their qualitative study, by using the tools of dynamical system theory, is presented.

Keywords: compact pairwise model, SIS epidemic, heterogeneous random networks

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MS30: Nonlinear diffusion processes: cross diffusion, complex diffusion and related topics

MS30: Nonlinear Diffusion Processes: Cross diffusion, complex diffusion and related topics

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Nonlinear diffusion equations have attracted a lot of attention over the last few years in many practical applications. After the pioneering work of Keler and Segel in the 1970s, cross-diffusion models became very popular in biology, chemistry and physics to emulate systems with multiple species. The range of application is even wider and, in particular, complex-diffusion models are of special relevance for example in the field of image processing. Meanwhile the underlying mathematical theory has been developed in a synergetic way with applications, in recent years, this topic became the focus of an intensive research within the mathematics community. In spite of the relevance of cross-diffusion models in numerous fields of application and all the mathematical activity around them, important questions remain unanswered and meaningful challenging problems still need to be addressed. The aim of this MS is to bring together researchers from the various fields, combining expertise in the theory of PDEs and competences in numerical analysis with a problem oriented perspective. The main goals are to give new insights in understanding the intimate nature of nonlinear processes, study their numerical discretizations, and develop sophisticated mathematical and computational tools that can be used efficiently in real problems, with special regards to cross diffusion and complex diffusion models. Motivations/relevance to ECMI In this symposium we gather scientists in pure and applied mathematics, computational science and physics with proven experience in the fields of computational biology and biomedical engineering, enhancing the visibility of recent developments in the topic of nonlinear cross-diffusion models.

Speakers:

A. Madzvamuse. The University of Sussex, School of Mathematical and Physical Sciences, Department of Mathematics, Brighton (United Kingdom). *Characterising the effects of cross-diffusion for reaction-diffusion models on stationary and evolving domains and surfaces.*

V. Selgas. Department of Mathematics, Universidad de Oviedo (Spain). *Analysis of a splitting-differentiation population model leading to cross-diffusion.*

L. Plociniczak. Wrocław, University of Technology, Wrocław (Poland). *Anomalous nonlinear diffusion in porous media: analytical approximations.*

A. Araújo. CMUC, Department of Mathematics, University of Coimbra (Portugal). *A Cross-diffusion models for image processing I. Linear case.*

A. Durán. Department of Applied Mathematics, University of Valladolid (Spain). *Cross-diffusion models for image processing II. Nonlinear case.*

C. Totzeck. TU Kaiserslautern (Germany). *Consensus-based global optimization.*

Characterising the effects of cross-diffusion for reaction-diffusion models on stationary and evolving domains and surfaces.

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I this talk, I will present linear stability analytical results of a two component reaction-diffusion system with linear cross-diffusion posed on continuously evolving domains (of which stationary domains will be a special case). First the model system is mapped from a continuously evolving domain to a reference stationary frame resulting in a system of partial differential equations with time-dependent coefficients. Second, by employing appropriately asymptotic theory, we derive and prove cross-diffusion-driven instability conditions for the model system for the case of slow, isotropic domain growth. Our analytical results reveal that unlike the restrictive diffusion-driven instability conditions on stationary domains, in the presence of cross-diffusion coupled with domain evolution, it is no longer necessary to enforce cross nor pure kinetic conditions. The restriction to *activator-inhibitor* kinetics to induce pattern formation on a growing biological system is no longer a requirement. Reaction-cross-diffusion models with equal diffusion coefficients in the principal components as well as those of the *short-range inhibition, long-range activation* and *activator-activator* form can generate patterns only in the presence of cross-diffusion coupled with domain evolution. To confirm our theoretical findings, detailed parameter spaces are exhibited for the special cases of isotropic exponential, linear and logistic growth profiles. In support of our theoretical predictions, we present evolving or moving finite element solutions exhibiting patterns generated by a *short-range inhibition, long-range activation* reaction-diffusion model with linear cross-diffusion in the presence of domain evolution. Furthermore, computational results on evolving surfaces will be discussed as part of the generalisation of the theory.

Keywords: Reaction-diffusion, cross-diffusion, linear stability analysis, pattern formation, asymptotic theory, cross-diffusion driven instability, domain-growth induced instability, finite elements, surface finite elements, evolving domains and surfaces

Acknowledgments. This work (AM) received funding from the European Union's Horizon2020 research and innovation programme under the Marie Sklodowska-Curie ITN grant agreement No 642866. AM also acknowledges support from the Engineering and Physical Sciences Research Council, UK grant (EP/J016780/1) and the Leverhulme Trust Research Project Grant (RPG-2014-149). Part of this work was undertaken when AM and RB were programme participants of the Isaac Newton Institute for Mathematical Sciences 6-months programme on *Coupling geometric PDEs with physics for cell morphology, motility and pattern formation* (13 July – 18 December 2015). The work (AM) was partially supported by a grant from the Simons Foundation. The bulk of this work was carried out while RB was a Visiting Scholar supported by the EPSRC grant (EP/J016780/1) to collaborate with AM.

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Analysis of a splitting-differentiation population model leading to cross-diffusion

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This work is motivated by the generalization to space dependent populations of the dynamical system model for the splitting-differentiation process of (space independent) populations proposed by Sánchez-Palencia in [5]. Indeed, such generalization leads to a family of cross-diffusion partial differential equations problems which include several well known segregation models.

Among these segregation models, in our previous article [3] we studied the case where the cross-diffusion is of the type introduced by Shigesada et al. in [6]. On the contrary, in this work we consider the model proposed by Busenberg and Travis in [2] and where we expect the the segregation effects to be stronger. See [4] and the references therein for further analysis of these models.

We propose a proof of existence of solutions which is conceptually simpler than the previous proof in [1]. Indeed, our proof is based on a direct parabolic regularization of the problem, whereas previous proofs involved a change of unknowns rendering the problem to a parabolic-hyperbolic formulation. Moreover, we believe that our approach also gives a way to select a unique natural solution of the problem as a limit of vanishing viscosity solutions of the regularized parabolic problems and, therefore, it overcomes the possible non-uniqueness issue of the parabolic-hyperbolic formulation.

For a deeper understanding of the numerical behaviour of our approach, we have introduced a Finite Element discretization of both our parabolic regularization and the formulation of [1], and then compared the results in a series of experiments. The general observation is that our approach is always more stable in the tricky regions where the solutions exhibit discontinuities. Finally, there are evidences in our numerical experiments showing that the main data restriction of the existence theorems (i.e. the positivity of the initial total mass) is not a necessary condition and may be weakened to non-negativity of the initial total mass.

Keywords: cross-diffusion system, population dynamics, contact inhibition, splitting and differentiation, numerical simulations, existence of solutions.
Acknowledgments. Partially supported by the Spanish MEC Project MTM2013-43671-P.

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Anomalous nonlinear diffusion in porous media: analytical approximations

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During the last few decades a rapid growth of methods and models based on differential equations of arbitrary order has been observed. This research is, as almost always, motivated in a twofold way - both by the pure mathematical curiosity and by physical phenomena, which adequate description is beyond the classical mathematical modeling.

My considerations are based on previously results [1, 2, 3]. The issue of anomalous diffusion has been present in literature for several years, especially when the diffusion is being described by a linear equation [4]. More precisely, the self-similar scaling for a problem of diffusion with conditions

$$u(x,0)=0, \quad u(0,t)=1, \tag{1}$$

is not equal to $x/\sqrt{t}$ but rather $x/t^{\alpha/2}$ for some $0<\alpha<2$. Here, $u=u(x,t)$ is the concentration of a substance being diffused at point x in time t. The fractional setting seems to be a very natural choice and so far has been very successful. This topic is being constantly developed but mostly on the grounds of numerical analysis. The main point of my research is the fractional partial differential equation modeling the anomalous diffusion

$$\partial_t^\alpha u(x,t)=\left(D(u)u_x(x,t)\right)_x, \tag{2}$$

where $D=D(u)$ is concentration-dependent diffusion coefficient and ∂_t^α is the fractional Riemann-Liouville partial derivative operator. Unfortunately equation (2) is hopelessly difficult to solve analytically. Even the numerical simulations are far from trivial. My strategy of finding an approximate solution of (2) is based on a power series approximation of the Erdelyi-Kober fractional operator

$$I_c^{a,b}U(\eta)=\frac{1}{\Gamma(b)}\int_0^1(1-z)^{b-1}z^aU(\eta z^{\frac{1}{c}})dz. \tag{3}$$

Further analysis reveals that the found series converges very quickly and to obtain a very reasonable approximation of $I_c^{a,b}$ it is sufficient to truncate the series after some one or two terms. As a result, the fractional equation transforms into an ordinary one which can be solved by approximate methods. The numerical verification of the various approximations confirms a very good accuracy of the method. Also, an application of these results to the description of anomalous diffusion gives very good results.

Keywords: anomalous diffusion, nonlocal equation, approximate solution

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A Cross-diffusion models for image processing I. Linear case

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Diffusion processes are commonly used in image processing [1]. In particular, complex diffusion have been successfully applied in medical imaging denoising [2]. The present talk will introduce the first part of a study on the use of cross diffusion systems to model different phenomena in image processing. The most common continuous representation of a grey-scale image is given by a real valued function standing for the grey-scale value of the image at the pixels. The use of two scalar fields may have the goal of distributing the features of the image and governing their relations. In this talk, the linear cross-diffusion filtering is discussed, in order to determine those kernels that ensure relevant scale-space properties to the model.

Keywords: cross-diffusion, image processing.
Acknowledgments. This work was supported by: project MTM2014-54710-P; the Centre for Mathematics of the University of Coimbra - UID/MAT/00324/2013; the Portuguese Government through FCT/MEC and the European Regional Development Fund through the Partnership Agreement PT2020.

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Cross-diffusion models for image processing II. Nonlinear case

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Diffusion processes are commonly used in image processing [1]. In particular, nonlinear complex diffusion have been successfully applied in medical imaging despeckling and denoising [2]. The present talk will introduce the second part of a study on the use of cross diffusion systems to model different phenomena in image processing. The use of two scalar fields may have the goal of distributing the features of the image and governing their relations. This second part will be devoted to study the effect of introducing nonlinearities in the system by way of a cross-diffusion matrix that depend on the image. Special attention will be given to the well-posedness and the scale-space properties of the model.

Keywords: cross-diffusion, image processing.
Acknowledgments. This work was supported by: project MTM2014-54710-P; the Centre for Mathematics of the University of Coimbra – UID/MAT/00324/2013; the Portuguese Government through FCT/MEC and the European Regional Development Fund through the Partnership Agreement PT2020.

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Consensus-based global optimization

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A consensus-based model for global optimization problems [1, 2] is presented and the differences to some other well-known methods are discussed. We shed some light on the prospects of justifying the efficacy of the optimization algorithm in the mean-field sense. Extensions of the mean-field equation to include non-linear diffusion of porous medium type is introduced. Theoretical results on decay estimates are then underlined by numerical simulations.

Joint work with: J.A. Carrillo, Y.P. Choi, S. Martin, R. Pinnau, O. Tse.

Keywords: Global optimization, opinion dynamics, consensus formation, agent-based models, stochastic dynamics, mean-field limit.
Acknowledgments. JAC was partially supported by the project MTM2011-27739-C04-02 DGI (Spain) and from the Royal Society by a Wolfson Research Merit Award. JAC and Y-PC were partially supported by the EPSRC grant EP/K008404/1. CT was partially supported by a Kurzzeitstipendium of the DAAD (German Academic Exchange Service).

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MS31: Mathematics for industry network (MI-NET) opportunities for participation

MS31: Mathematics for Industry Network (MI-NET) – opportunities for participation

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The Mathematics for Industry Network promotes partnerships between mathematicians and industrialists www.mi-network.org.

Over the next four years, funded by an EU COST Action, MI-NET will support a pan-European programme of networking activities in industrial maths across over 30 countries.

MI-NET is an open network, so there are still many opportunities for researchers - in particular those at early stages of their careers - to get involved. This minisymposium will raise awareness of the benefits of joining the network, planned networking events, and the funding available for industrial maths activities.

The speakers in this minisymposium, each from different MI-NET countries, will showcase the MI-NET vision and describe their own experience of hosting modelling weeks, industrial workshops, and participating in research visits.

J. Jordan. Bath Institute for Mathematical Innovation, University of Bath (UK). *Introducing the Mathematics for Industry Network (MI-NET).*

V. Rottschafer. Leiden University (Netherlands). *Bringing companies and mathematicians together via European Study Groups with Industry.*

T. Ivanov. Sofia University (Bulgaria). *Modelling weeks in the MI-NET framework.*

K. Kaouri. Cyprus University of Technology (Cyprus). *Research visits.*

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Introducing the Mathematics for Industry Network (MI-NET)

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The Mathematics for Industry Network promotes partnerships between mathematicians and industrialists www.mi-network.org. During 2015-2019, funded by an EU COST Action, MI-NET will support a pan-European programme of networking activities in industrial maths across over 30 countries.

In this talk, I will outline the MI-NET vision, the benefits of joining the network, planned events, and the funding available for industrial maths activities.

Acknowledgments. The Mathematics for Industry Network COST Action TD1409 is supported by COST (European Cooperation in Science and Technology) via the EU Framework Programme Horizon 2020

Bringing companies and mathematicians together via European Study Groups with Industry

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European Study Groups with Industry (ESGIs) are combined industrial/academic workshops where mathematics is used to tackle problems presented by companies and other organisations outside academia. Between fifty to eighty mathematicians from a wide range of backgrounds, both from industry and academia, gather during the week to collaborate intensively on industrial problems, see [1]. In this talk, I will address the benefits of participating in an ESGI for both the companies and the academics, and present several success stories of Dutch ESGIs.

ESGIs have been organised in the Netherlands since 1998, see [2] for the website of the Dutch ESGIs. The format follows the original Oxford model, dating back to 1968, which is used worldwide in similar study groups. On the Monday the industrial representatives outline their project and their objectives. The participants devote the entire week to brainstorming, modelling and solving these problems in smaller groups. During the week the groups maintain contact with the problem owners to ensure that their efforts stay targeted at the problems posed by the companies. All groups present their work on the Friday morning. After the week, a report is written for the company and this is also published as the scientific proceedings. In the Netherlands, we also hire a professional technical writer to write popular proceedings that are targeted at a general audience.

The success of the ESGIs is demonstrated by the extent to which the unique format has been copied around the world and is now extending into other areas where mathematics may be applied. Through MI-NET we aim to increase the number of European countries in which ESGIs are organised.

Keywords: Study Group.

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Modelling weeks in the MI-NET framework

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Modelling weeks are internationally recognized forums that have been incorporated in the ECMI philosophy for education in Industrial Mathematics for a long time [1]. They gather together students having various backgrounds and usually coming from different countries. Participants work intensively in a period of 5-7 days, divided into groups of 5-6 people each in order to propose a solution of a relevant practical problem that could be approached by the tools of Mathematics. For this purpose, they are guided by an instructor who is experienced in working on applied projects and in the field of the problem, in particular.

Thus, modelling weeks serve several main objectives:

- to introduce students to mathematical modelling and working on real-life problems;
- to train students in working in multinational environment, collaborating and communicating ideas with different people, coming from different backgrounds;
- to train students in presenting their results.

MI-NET (Mathematics for Industry Network, [2]) is a COST funded project that during its lifetime will be supporting several modelling weeks, focused mainly on PhD level, every year. Possibilities for participating by prospective organizers will be presented.

Several important topics in the organization and carrying of a modelling week will be discussed taking into account the points of view of students, instructors, and organizers, e.g. choosing appropriate projects, forming teams, organizational and financial matters, etc.

The benefits of participating in a modelling week will be commented on by presenting several success stories of students with results, achieved as a direct result of their participation in a modelling week.

Keywords: Modelling weeks, Funding possibilities, Education in Industrial Mathematics
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Research visits

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In this talk, I will outline the opportunities for Short Term Scientific Missions (STSMs), research visits which are available within the COST Action TD1409 "Mathematics for Industry Network"[1] (MI-NET). Furthermore, I will relay my experience from a recent research visit at the University of Oxford, which also involved receiving training in establishing a European Study Group with Industry [2], and in further developing industrial mathematics in Cyprus.

Keywords: Research Visit, Industrial Mathematics, Networking, COST Action

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MS33: Mathematical modeling and numerical simulation in controlled drug release

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Mathematics is playing an increasing role in the field of medicine through the use of models and numerical simulations. These models represent an extremely useful tool to complement theoretical and experimental work and provide personalised models for patient treatment.

Drugs had a main role in improving health and extending lives, but drug delivery systems have changed in a very impressive manner during the last decades. Controlled drug delivery systems, as drug eluting stents, transdermal patches, intravitreal implants, targetted systems for antitumor drug release, have became nowadays a common tool in clinical practice. These drug delivery systems combine a platform with a drug in a such way that the active agent is efficiently released to a target organ, while maintaining the drug concentration within a therapeutic window during an extended period of time. Devices and drugs can be tuned to meet the individual patient needs.

This symposium aims to promote an interdisciplinary forum for sharing the new ideas that will shape the role of mathematical modeling and numerical simulation in a third generation healthcare. Contributions that can have a direct impact on patient care at all the different stages of healthcare -diagnosis, treatment and drug delivery - are welcome.

Speakers:

J. R. Branco. CMUC & Polytechnic Institute of Coimbra, ISEC, DFM, Coimbra (Portugal). *A mathematical look at chemotherapy protocols for brain tumours.*

J. A. Ferreira. CMUC, Department of Mathematics of University of Coimbra (Portugal). *Drug release from viscoelastic polymeric platforms.*

G. Pena. CMUC, Department of Mathematics, University of Coimbra (Portugal). *Mathematical modelling, analysis and simulation of an iontoforetic drug delivery device.*

J. Naghipoor. Institute of Structural Mechanics, Bauhaus University of Weimar (Germany). *The effect of atherosclerotic plaque on the drug eluted from bioabsorbable stents.*

Keywords: Mathematical modeling, numerical simulation, controlled drug release.
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A mathematical look at chemotherapy protocols for brain tumours

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Tumours are the uncontrolled growth of abnormal cells. Gliomas, which are a special case of brain tumours, have a high mortality rate, giving six months to one year of life expectancy once its diagnosed in patients (even undergoing treatment). Medical doctors believe that a reason for the inefficiency of such treatments lies in the high motility of the tumour cells.

The modelling of migration and proliferation of tumour cells has received attention by the scientific community in the last decades. A possible approach is to model the motion of tumour cells by passive diffusion. This was first proposed in [5], who introduced a partial differential equation built upon a mass conservation law. Later work by [3, 4], based on the principles followed by [5], modelled tumour cells as having two possible phenotypes (or states), proliferative and migratory, allowing cells to transition between both phenotypes.

The study of treatment protocols, based upon the partial differential systems that model chemotherapy effects in tumour growth, has also received some attention recently. In [1], the authors deduced, for a linear problem, bounds for different energies of the system. This allowed to show, under suitable sufficient conditions, the regression of the tumoral mass, thus creating the possibility of defining treatment protocols. A more complex model was proposed in [2], introducing nonlinear terms for the coupling between drug concentration and tumour cells' removal.

In this talk we introduce the a nonlinear model for the evolution of tumour cells and concentration of chemotherapy drug based in mass conversation laws. This model is an extension of the model proposed in [2] by adding integral terms to account for the rigidity of the brain tissue. The stability of the solution of the nonlinear system shall be addressed. In order to define treatment protocols, the study of the mass of cells will lead to relations between the treatment parameters that allow to control the size of the tumour. Finally, some simulations illustrating the obtained results will be explored.

Keywords: Glioma, chemotherapy, numerical simulation.
Acknowledgments. This work was partially supported by the Centre for Mathematics of the University of Coimbra – UID/MAT/00324/2013, funded by the Portuguese Government through FCT/MEC and co-funded by the European Regional Development Fund through the Partnership Agreement PT2020.

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Drug release from viscoelastic polymeric platforms

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Polymeric drug delivery platforms are nowadays of common use because they can be designed with prescribed properties that lead to an optimized drug release. The drug is initially dispersed in the polymeric network and when the platform enters in contact with a solvent fluid a set of complex phenomena occur. The sorption of the fluid takes place and the polymer swells. The liquid strains the polymeric matrix that, while swelling, exerts a stress that acts as a barrier to the incoming fluid. To explain these phenomena several authors agree that a non Fickian solvent mass flux depending on the strain must be considered. Without being exhaustive we mention [1],[2], [3] [4] [5] and [6].

The aim of this work is to study the drug release from a spherical viscoelastic polymeric platform where a drug is initially dispersed. The device is inside of another sphere with a resident solvent fluid. We assume that (i) the polymeric platform swells upon contact with the resident solvent; (ii) the viscoelastic behaviour is described by a generalized Maxwell-Wiechert model; (iii) the viscoelasticity induces a resistance to the solvent uptake; (iv) drug dissolution and Fickian drug diffusion take place in the swollen polymer (v) drug diffusion occurs in the spherical surrounding sphere.

The drug release is described by a system of PDE's defined in a time dependent domain: an integro-differential equation for the absorbed solvent, a diffusion equation for the released drug, a reaction equation for the undissolved drug. This system is coupled with a drug diffusion equation in the surrounding domain. The two problems are complemented by interface, boundary and initial conditions. The mathematical model is studied from an analytical and numerical point of view.

Keywords: Viscoelastic polymeric drug delivery device, Fickian diffusion, non-Fickian diffusion
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Mathematical modelling, analysis and simulation of an iontoforetic drug delivery device

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Intelligent drug delivery devices have been developed during the last decades to deliver drugs in a controlled manner at specific locations. Some of these systems use stimuli-responsive polymers (where the drug is entrapped) that are able to respond to the modification of the external environment (like electric fields, pH and temperature). Electric fields are an interesting type of stimulus because they can be precisely controlled, and the drug delivery responses can be predicted.

The use of electric fields as enhancers is popular in transdermal drug delivery where iontophoresis ([3, 4]) and electroporation ([1, 2]) or a combination of both, are usual procedures. Drug delivery systems for cancer treatment based on this technology were recently developed ([6]). In this case, the device based on drug-encapsulated nanoparticles is remotely controlled by an electric field to deliver the biological agent in the cancer target tissue (electrochemotherapy, see [5]).

In an iontophoretic procedure, a small electric field is applied to the coupled system to enhance the drug transport. The generated electric field induces a convective flux in the system that depends on the drug molecules valence, intensity of the electric field, temperature, electric conductivity of both media and drug diffusion ([3, 4]).

In this talk we study a simplified one dimensional drug delivery mechanism from a reservoir which is in (perfect) contact with the skin. We assume that the drug transport in the coupled system is enhanced by a small electric field that induces a convective field. We establish energy estimates for the coupled system and we propose a semi-analytical discrete coupled model that mimics the continuous one. The qualitative behaviour of the system is illustrated.

Keywords: iontoforesis, drug release, finite differences, energy estimates.
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The effect of atherosclerotic plaque on the drug eluted from bioabsorbable stents

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Atherosclerosis in the coronary artery is one of the leading causes of the death in the world. Balloon angioplasty with stenting as a non-invasive technique is considered as a well established and effective tool to reduce the severity of atherosclerotic stenosis. A common problem called in-stent restenosis is the main drawback of the stenting in the coronary artery. Having information about the spatial and temporal drug release from drug-eluting stents and drug uptake in the arterial wall could be a useful tool to investigate in-stent restenosis growth which is experimentally expensive to study.

Mathematical modeling together with numerical simulation facilitates the improvement of stent efficacy by understanding its functionality ([1]–[5]). In this work, the local delivery of a therapeutic agent from a PLA based bioabsorbable stent implanted in a coronary artery is mathematically modeled and numerically simulated to investigate on the drug release and spatio-temporal drug distribution in different plaques. The mathematical model is represented by two coupled systems of PDE's that describe the pharmacokinetics of drug in the stent and the diffusion of the drug with reversible binding in the viscoelastic arterial wall. The effect of plaque composition, on the accumulation of drug released by a drug eluting stent, is analyzed. The influence of the stiffness and porosity of the soft and hard plaques is studied. A case study based on OCT images is also included.

Keywords: Atherosclerosis plaque, porosity, viscoelasticity, drug eluting stent, numerical simulation.
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MS34: Mathematical modeling of charge transport in graphene and low dimensional structure

MS34: Mathematical modeling of charge transport in graphene and low dimensional structure

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The minisymposium will be concerned with the mathematical modeling and simulation of charge transport in graphene and other 2D materials and in structures, like double gate MOSFETs, nano-ribbons and nano-wires, where the presence of confinement effects allows for the formal description of the carrier flow as that of a two dimensional or one dimensional electron gas. Graphene, thanks to its peculiar electrical properties and mechanical properties, is considered as one of the most promising materials for future electron devices. Lately, it has also been realized that, by increasing the miniaturization of devices, hot-spots are observed, that is zones with very high crystal temperature due to the release of energy by high energetic electrons. The effect is particularly relevant in materials with reduced dimensionality and confined structures. For these reasons, the mini symposium will foresee the discussion of the following arguments: ab initio calculations to furnish the correct band structures for the materials, e.g. doped graphene or graphene nanoribons; thermal effects in the crystal lattice; analytical properties of the Schroedinger equation; Monte Carlo simulations; Wigner transport equation; numerical schemes for the charge carrier transport equation; fluid models deduced from the kinetic transport equations.

Speakers:

G. Mascali. Università della Calabria and INFN-Gruppo c. Cosenza (Italy). *Semiconductor thermal conductivity and how it is affected by embedding nanoparticles.*

F. Vecil. Université Blaise Pascal (France). *Implementation on a high-performance computing platform of a deterministic solver for Double-Gate MOSFETs.*

V. Romano. Universiy of Catania (Italy). *Deterministic and stochastic solutions of the Boltzmann equation for charge transport in graphene on substrates.*

O. Muscato. Universiy of Catania (Italy). *Low-field electron mobility in silicon nanowires obtained via hydrodynamic simulations.*

A. La Magna. IMM-CNR, Stradale Primosole, Catania (Italy). *Atomistic dynamics and electronic transport in hydrogenated graphene.*

I. Deretzis. IMM-CNR, Stradale Primosole, Catania (Italy. *Selective band structure unfolding for the determination of the p-type character of oxygen-treated few-layer MoS2.*

G. Alí. Università della Calabria (Italy). *Some analytical results for a two-temperature energy-transport model for semiconductors.*

N. Rotundo. WIAS Berlin (Germany). *On some extension of energy-drift-diffusion models.*

Keywords: electron transport, graphene, 2D electron gas, quantum transport, electron devices.

Semiconductor thermal conductivity and how it is effected by embedding nanoparticles

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Heat conduction in semiconductors and insulators has been object of extensive experimental and theoretical studies [1, 2, 3, 5, 4], since heat removal has become a crucial issue in modern electronic devices, due to the increased levels of dissipated power density and speed of electronic circuits. In this type of materials, energy is essentially carried by phonons, in particular the acoustic ones, therefore in order to understand the behavior of conductivity, it is essential to study the transport of phonons considering the fundamental scattering mechanisms to which they are subject.
In this work, starting from the kinetic description based on the Callaway approximation of the phonon collision operator [1], we develop a hierarchy of macroscopic models in which the state variables of the acoustic phonons are moments of their occupation numbers. The evolution equations for these macroscopic variables are found by integration from the Boltzmann equations and they are closed on the basis of the maximum entropy principle [4]. Exploiting these equations, we show that it is possible to derive a new formula for conductivity, which, if a sufficient number of moments is used, allows us to recover all the results of the Callaway formula in the steady-state [1], and to obtain findings in agreement with those in [2] in the dynamical case.
In particular, the formula is able to predict the effect of embedding nanoparticles in alloy crystals like InGaAs or SiGe. In fact, it is confirms that the steady-state thermal conductivity is reduced at the increase of the nanoparticle radius, while the cutoff frequency f_C of the dynamical conductivity is increased with respect to the intrinsic alloys. Both these effects could be very advantageous in many microelectronic and optoelectronic device applications. In particular, reducing thermal conductivity is crucial in order to improve the efficiency of solid-state thermoelectric converters and make them competitive with the traditional electric generators or refrigerators.

Keywords: Semiconductors, Lattice conductivity, Hydrodynamical models, Maximum Entropy Principle, Nanoparticles.
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Implementation on a high-performance computing platform of a deterministic solver for Double-Gate MOSFETs

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The Double-Gate MOSFET is a widespread transistor type. Its evolution has witnessed a constant downscaling, from the 10000 nm of the Seventies to the 14 nm of nowaday's smallest MOSFET on the market. Downscaling is important for both better performances and saving of silicon and energy. We simulate a 10 nm device using a hybrid, deterministic, high-dimensional model, so as to fulfill two main goals: being a benchmark for the accuracy other faster but coarser solvers (hydrodynamic, Monte-Carlo, SHE); providing reliable information on zones with a weak amount of charge, something that Monte-Carlo-based simulations cannot do. As a sequential, one-core simulation takes about one month, a parallelization on the graphic card is being realized. We shall show the results obtained until now and a comparison to Monte-Carlo [1, 2].

Keywords: MOSFET device, Boltzmann equation, Schrödinger equation, dimensional coupling, GPU.
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Deterministic and stochastic solutions of the Boltzmann equation for charge transport in graphene on substrates

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A physically accurate model for charge transport in graphene is given by a semiclassical Boltzmann equation whose scattering terms have been deeply analyzed in the last decade. Due to the computational difficulties, the most part of the available solutions have been obtained with direct Monte Carlo simulations. The aim of this work is to simulate a monolayer graphene on a substrate, as, for instance, considered in [3].
We use a numerical scheme based on the discontinuous Galerkin method for finding deterministic (non stochastic) solutions of the electron Boltzmann equation in graphene [4]. The results are compared with those obtained with a recent DSMC approach that properly takes into account the Pauli exclusion principle [4].
In a semiclassical kinetic setting, the charge transport in graphene is described by four Boltzmann equations, one for electrons in the valence (π) band and one for electrons in the conductions (π^*) band, that in turn can belong to the K or K' valley,

$$\frac{\partial f_{\ell,s}(\mathrm{t},\mathbf{x},\mathbf{k})}{\partial t} + \mathbf{v}_{\ell,s}\cdot\nabla_{\mathbf{x}} f_{\ell,s}(\mathrm{t},\mathbf{x},\mathbf{k}) - \frac{e}{\hbar}\mathbf{E}\cdot\nabla_{\mathbf{k}} f_{\ell,s}(\mathrm{t},\mathbf{x},\mathbf{k}) = \left.\frac{df_{\ell,s}}{dt}(\mathrm{t},\mathbf{x},\mathbf{k})\right|_{e-ph},$$

where $f_{\ell,s}(\mathrm{t},\mathbf{x},\mathbf{k})$ represents the distribution function of charge carriers in the valley ℓ (K or K'), band π or π^* ($s=-1$ or $s=1$) at position $\mathbf{x}$, time t and wave-vector $\mathbf{k}$. We denote by $\nabla_{\mathbf{x}}$ and $\nabla_{\mathbf{k}}$ the gradients with respect to the position and wave-vector, respectively. The microscopic velocity $\mathbf{v}_{\ell,s}$ is related to the energy band $\varepsilon_{\ell,s}$ by

$$\mathbf{v}_{\ell,s} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\,\varepsilon_{\ell,s}\,.$$

With a very good approximation [1] a linear dispersion relation holds for the energy bands $\varepsilon_{\ell,s}$ around the equivalent Dirac points; so that $\varepsilon_{\ell,s} = s\,\hbar\,v_F\,|\mathbf{k}-\mathbf{k}_\ell|$, where v_F is the (constant) Fermi velocity, $\hbar$ is the Planck constant divided by $2\,\pi$, and $\mathbf{k}_\ell$ is the position of the Dirac point ℓ. The elementary (positive) charge is denoted by e, and $\mathbf{E}$ is the electric field. The right hand side of the Boltzmann equation is the collision term representing the interaction of electrons with impurities and phonons, the latter due to both the graphene crystal and substrate [2]. We assume that phonons are at thermal equilibrium.
The main differences between graphene on a substrate and the suspended case are highlighted.

Keywords: charge transport, graphene, Discontinuous Galerkin, DSMC
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Low-field electron mobility in silicon nanowires

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Silicon nanowires (SiNWs) are quasi-one-dimensional structures in which electrons are spatially confined in two directions and they are free to move in the orthogonal direction. The subband decomposition and the electrostatic force field are obtained by solving the Schrödinger - Poisson coupled system. The electron transport along the free direction can be tackled using a hydrodynamic model which has been obtained by taking the moments of the multisubband Boltzmann equation, where explicit closure relations for the fluxes and production terms have obtained by means of the Maximum Entropy Principle of Extended Thermodynamics, including scattering of electrons with phonons [1, 2, 3] and surface roughness scattering.

In this paper, using this Schrödinger - Poisson - hydrodynamic model, we calculate the diffusive-regime low-field electron mobility which is one of the most important parameters that determines the performance of field-effect transistors (FETs), thermoelectric (TE) coolers, and sensors.

Keywords: nanowires, silicon, hydrodynamic.

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Atomistic dynamics and electronic transport in hydrogenated graphene

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The electronic structure of graphene can be greatly modified by hydrogen (H) absorption, leading to different electronic transport properties with respect to the non-functionalized material. However, the electron transport features of hydrogenated graphene could be significantly affected by the atomistic configurations dynamically formed during the hydrogenation, as well as from the eventual subsequent annealing processes. These dynamics are, in general, modified by the process parameters.

We have simulated the dynamics of hydrogen adatoms absorbed on top of graphene, using the Kinetic Lattice Monte Carlo (KLMC) approach [1], which allows us to stochastically study large time and space scales. The obtained structures are discussed and their quantum transport properties are investigated using Non-equilibrium Green Function (NEGF) calculations.

The hydrogenation process of graphene is simulated by a statistically ordered sequence of events modeling the local time-dependent modifications of the system during the processes. These modifications include H adsorption/desorption and surface diffusion of H adatoms adsorbed on top of graphene. We model diffusion, as a thermally activated process, which needs to overcame an energy barrier given by the sum of a migration energy and a short-ranged H-H adatom interaction energy, accounting for the stability of the local configurations. As a consequence, the event rate is given according the transition state theory by the Boltzmann weight $\nu_i = \nu_i^0 \exp\left[-E_i^{act}/kT\right]$, where E_i^{act} is the the activation energy barrier and ν_i^0 the frequency pre-factor. E_i^{act} is evaluated using an interaction energy model which depends only on the coordination of the adatoms, extending up to third nearest neighbors $E_i^{act} = E(n_1, n_2, n_3)$ and it is tested against the Density Function Theory (DFT). Atomic and associative desorption of hydrogen adatoms are also considered and corresponding energy barriers are estimated with the aid of *ab inito* computations, while atomic absorption occurs at a constant rate, fixed by an effective external atomic flux.

We model the quantum electron transport in the hydrogenated configurations simulated by KLMC considering a two-terminal resistor geometry including contacts. The electron hamiltonian H_0 is approximated by the tight-binding model of graphene where the hopping integrals to the sites occupied by the H adatoms are set to zero. The transport characteristics are calculated after the evaluation of the Green function G(E) from the matrix equation $G(E)[EI - H_{tot}] = I$, where E is the energy and H_{tot} is the total effective hamiltonian of the device including the two self-energy terms due to the contacts.

The main results of our combined KMLC-NEGF methodology can be outlined as follows: (a) H atoms reorganize in complex structures after the deposition and (eventual) annealing due to effective H-H interaction, and (b) the final configurations critically depend on the accuracy of the H-H model implemented to recover the DFT-calculated energetics. The conductance calculated by the NEGF is generally larger with respect to that obtained with a random distribution of H or using less accurate H-H interaction models. In conclusion, *ab inito* calibrated KLMC-NEGF simulations are used to predict the results of manipulation processes in hydrogenated graphene. This fully atomistic approach for the process/device simulation demonstrates its great potential when applied to two-dimensional materials.

Keywords: graphene, kinetic Monte Carlo, quantum transport

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Selective band structure unfolding for the determination of the p-type character of oxygen-treated few-layer MoS_2

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Albeit its excellent electrical properties, the use of graphene in digital devices and applications has been hindered by the absence of an intrinsic band-gap. This aspect has encouraged research on two-dimensional materials beyond graphene, like the transition metal dichalcogenides. Belonging to this family of materials, MoS_2 has demonstrated a particular potential for integration in thin-film transistors due to its tunable band-gap and its mechanical stability down to the single-layer level. As with traditional semiconductors, prior to using MoS_2 as a channel material, either n- or p-type doping has to be applied, with the later being a non-negligible problem. Nonetheless, it has been recently demonstrated that partial oxidation of MoS_2 gives rise to a tunable p-type doping [1, 2].

The objective of this study is to understand the origins of this behavior from a theoretical viewpoint, using the density functional theory. We initially show that both substitutional and interstitial oxygen atoms in MoS_2 systems are neutral defects, as they neither give rise to significant charge-transfer phenomena nor they insert defect states within the MoS_2 bandgap. We then employ an advanced computational methodology in order to unfold the bands of partially oxidized trilayer MoS_2 systems, considering the spatial contribution of each layer in the total electronic structure. The algorithm is based on the calculation of the spectral weight for each band, defined as [3]:

$$W_{\mathbf{k}} = \frac{1}{\mathcal{N}} \sum_{a \in PC} \left(\sum_{j}^{\mathcal{N}} \tilde{c}^{a+j}(\mathbf{k}) \right) \times \left(\sum_{j}^{\mathcal{N}} c^{a+j}(\mathbf{k}) \right) \tag{1}$$

where $\mathcal{N}$ is the number of elementary cells within the supercell, $c(\mathbf{k})$ are the expansion coefficients of the wave functions and $\tilde{c}(\mathbf{k})$ are coefficients that take into account the presence of a non-orthogonal basis set for the description of the system Hamiltonian [3].

Results show that if the oxygen-functionalization is confined in one out of the three layers of the system, the increase of the doping percentage gives rise to a gradual reduction of the Schottky barrier height for the valence band and a respective acquisition of a p-type character for the entire system. Based on the unfolding analysis, we observe a significant band misalignment between the doped and the undoped regions, with the former having a tendency to shift its bands towards lower energies. The picture extracted from our calculations indicates that such band misalignment, in conjunction with the absence of significant charge transfer effects is at the origin of the p-type behavior observed experimentally.

Keywords: MoS_2, density functional theory, band structure unfolding

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Some analytical results for a two-temperature energy-transport model for semiconductors

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By reducing the characteristic size to nanoscale dimensions, the effects of crystal heating have became crucial for the design of electron devices due to the possibility of having hot spots, that is, zones where the temperature of the lattice is very high, even close to the melting one. This has increased the interest on the analysis of thermal effects in semiconductors and prompted the formulation of improved models. Recently more sophisticated energy-transport models, based on closure relations obtained by employing the maximum entropy principle, have been proposed, e.g. [1], and used for simulating electron devices [2, 3]. The main features of these models is to include an additional variable representing the lattice temperature and a relative equation for that. The scattering mechanisms force equilibrium between the electron and lattice temperature. In turn the latter tends to an equilibrium state with the environment. The simplest way to take into account such a physical effect is with a relaxation time approximation involving two relaxation times, one for the electron-phonon interaction and another for the phonon-environment interaction.

From a mathematical point of view one has a standard energy-transport model augmented with a balance equation for the lattice temperature. We consider the (scaled) system:

$$\partial_t n + \nabla \cdot j = 0, \tag{1a}$$

$$j = n\nabla\phi - \nabla(nT), \tag{1b}$$

$$\partial_t \left(\frac{3}{2} nT\right) + \nabla \cdot \left(\frac{5}{2} Tj - \kappa_0 \nabla T\right) = j \cdot \nabla\phi - \frac{3}{2\tau} n(T - T_L), \tag{1c}$$

$$\partial_t (\rho c_V T_L) + \nabla \cdot (-\kappa_L \nabla T_L) = \frac{3}{2\tau} n(T - T_L) - \frac{1}{\tau_L}(T_L - 1), \tag{1d}$$

$$\nabla^2 \phi = n - D, \tag{1e}$$

with $x \in \Omega \subset \mathbb{R}^n$, n electron density, j current density, T electron temperature, T_L lattice temperature, ϕ electrostatic potential. κ_0 and κ_L represent the thermal conductivity of electron and lattice heat flux, τ and τ_L are the relaxation times for electron and lattice energy. D denotes the doping profile.

System (1) is the simplest energy-transport model with varying lattice temperature. For this system we prove an existence and uniqueness result.

Keywords: energy-transport models; semiconductors; existence and uniqueness.

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On some extension of energy-drift-diffusion models

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In this talk we discuss a hybrid modeling approach for the coupling of the classical energy-drift-diffusion models for heat and carrier transport in optoelectronic devices to quantum mechanical based microscopic models for the embedded low-dimensional nanostructures. Such type of models have been introduced in [1], which include a multi-species description for the carriers along the optically active region in QD lasers. Similar approaches have been proposed in [2] for the embedding of models for quantum well and quantum wire structures in to drift-diffusion models.

A consistent mathematical modeling for these extended energy-drift-diffusion systems is possible in the GENERIC (General Equations for Non-Equilibrium Reversible Irreversible Coupling) framework [4] and generalized gradient flows [5]. We will describe how the GENERIC framework is used to derive thermodynamically consistent coupled field equations, where the physical structure of the problem is well separated into reversible effects, driven by the free energy, and dissipative effects, driven by free entropy.

Keywords: optoelectronic devices, extended energy-drift-diffusion models, GENERIC framework, generalized gradient flows.
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MS35: Effective solutions for industry using mathematical technology

MS35: Effective solutions for industry using mathematical technology

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The main aim of this symposium is to present five of the most successful projects of ITMATI (Technological Institute of Industrial Mathematics) oriented to industrial customers, as a result of an intense relationship with our environment since our formal origin in February 2013, focusing in win-win engagements with all our stakeholders. We focus in projects developed from specific needs of companies, reason of our conviction to promote the Transference of Applied Knowledge to the Industry. Specifically,

- to facilitate and promote the application of mathematical techniques and methods in the productive sector,
- to develop new technological knowledge to improve the competitiveness of the companies in the field of technology and innovation,
- to provide services of support to business innovation,
- to spread the technological knowledge of the ITMATI,
- to boost academic and scientific collaborations with universities and centres of research and transfer and enhance interdisciplinary,
- to help strengthen the relationship between source of knowledge and business.

This minisymposium emphasizes the importance of this mathematical transference applied to the resolution of industrial problems. In particular, five success stories between research groups in industrial mathematics and companies are presented. Namely:

Part 1: Applied Mathematics

- A. Souto-Serantes. FerroAtlántica, Spain. *The mathematical modeling in the R & D Department of FerroAtlántica*

  Several projects have been undertaken in recent years that have led to exchanges with leading research centers and universities around the world. We have chosen as an example for this session the Electromagnetic casting furnace model (EMC) where the electromagnetic and thermodynamic model was done in detail. We will expose its results and the consequences of them on the industrial project.

- Svenn Anton Halvorsen. Teknova AS, Norway. *Practical industrial mathematics – between industry and academia.*

  Metallurgical Scale-up project include general thermal and electric scale-up, with application for electrodes and slag furnaces. The examples show that mathematical modelling is a very valuable tool to study metallurgical processes. Good cooperation between industry and academia, combining industrial experience, metallurgy and mathematics is mandatory.

- J. García San Luis, J.F. Rodríguez Calo. Repsol Technology Center, Spain. *Fostering successful partnerships between industry and academia. ITMATI-Repsol research center.*

  In the joint research unit Repsol-ITMATI, the company Repsol pursues a competitive advantage in dealing with different problems of mathematical programming, and tries to obtain that advantage by developing and implementing mathematical and computational methods in software tools, with immediate application in their business units.

Part 2: Statistics and Operations Research

- K. Wuerzburg, A. Casal. Inova, Spain. *Applications of smart data management and analytic systems in the maritime industry.*

  InovaLabs has successfully applied data management techniques in maritime industries, helping companies to implement energy efficient and intelligent systems. Two of these systems are a demand forecast tool for an innovative clean power supply for seagoing vessels at port, and an intelligent decision support tool to predict and analyse the impact of energy-efficient and emission reduction measures at port infrastructure .

- A. Lorenzo, J.L. Sáiz. INAER, Spain. *Mathematics in the service of emergencies.*

  INAER is an enterprise of the Babcock group that provides air services, including air services in emergencies such as wildfire, medical emergencies, search and rescue missions. Acquiring data will not suffice: the cornerstone of the progress forward will be developing the capacity for processing all this data and obtain reliable information, sometimes in real time. We can distinguish three main lines of work: process and fusion of spatial data from the surface of the Earth related to properties of the terrain or the surface of the sea, process of geolocation data in real time and, after action, statistical analysis of mission data.

Mathematical models in the R & D department of FerroAtlántica

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In the last 20 years, the R & D Department of FerroAtlántica has requested the mathematical modeling of almost all their industrial projects. These models has been developed by means of an extensive collaboration with the Department of Applied Mathematics of the University of Santiago de Compostela (Spain). The engineers of the company and the researchers of the university created a multidisciplinary team which was essential to understand the difficulties of each project and interchange useful information. In particular, the company provided all the data needed for the simulations and even installed specific measure tools in the plant to validate the numerical results. An important number of research projects have been developed in this framework and derived in several doctoral thesis, journal publications and relevant collaborations with international research centers and universities; see, for instance, [1, 2, 3, 4, 5, 6].

In this presentation, we will focus on the electromagnetic and thermodynamic modeling of an electromagnetic casting furnace (EMC). We will present the numerical results obtained and their impact in the development of the industrial project.

Keywords: Silicon, Solar silicon, Mathematical models, Electromagnetic casting.

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Practical Industrial Mathematics – Between Industry and Academia

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Teknova is a small research institute located in the southern part of Norway. We collaborate closely with several metallurgical companies, among others, within industrial mathematics. Industrial problems are normally interdisciplinary, can be very challenging, and many factors are required to succeed:

- *Trust* – Industial information is essential, and the company must trust that it will not be misused.
- *Technical competence* – Within the relevant fields, to fully understand the industrial jargon.
- *Broad mathematical competence* – To do proper mathematical modelling.
- *Translator skills* – The ability to "translate" the industrial problem to a mathematical model, and interpret the model results in a language understood within the industrial company.
- *Network* – Know who can be consulted whenever own competence needs to be supplemented.

Cases from two major projects at Teknova will be discussed, *Metallurgical Scale-up* and *Electrical Conditions in Metal Processes (ElMet)*. Both projects include mathematical expertise from University of Oxford and University of Santiago the Compostela (USC), in addition to excellent metallurgical competence from The Norwegian University of Science and Technology (NTNU) and Norwegian metallurgical companies.

Metallurgical Scale-up ended last year. Here, we have mainly demonstrated how comparatively simple mathematical analysis can supply valuable scale-up information. The studies include general thermal and electric scale-up, with application for electrodes and slag furnaces. [1]

The ElMet project started last year, and will continue through 2019. Previous simulations within metallurgy have often applied direct current (DC), to study large, 3-phase, smelting furnaces. Such DC simulations are valid for "only one instant of time" [2]. It is not straightforward to interpret the results for real furnaces. Within ElMet we have shown that an approximate harmonic solution for 3-phase alternating currents (AC), can be described as a superposition of three DC solutions, taking the phase shift between the three electrodes into account [3]. The problem will be brought to a European Study Group with Industry (ESGI) in Santiago de Compostela, September 2016, with the intention to compare our approximation with full electromagnetic simulations. Our AC approximation is valid for small furnaces. We now want to clarify how well it works for large ones.

The examples show that mathematical modelling is a very valuable tool to study metallurgical processes. Good cooperation between industry and academia, combining industrial experience, metallurgy and mathematics is mandatory. In this setting, the translator role should not be underestimated.

Keywords: Mathematical modelling, Metallurgy, Translator.
Acknowledgments: The projects has been funded by Regional Research Fund Agder, The Research Council of Norway, as well as major Norwegian metallurgical companies.

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Fostering successful partnerships between industry and academia. ITMATI-Repsol research center

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ABSTRACT

Last decade has seen a remarkably increasing pace in technological change. Moreover, technological disruptions are often related to a conjunction of different technical disciplines with increasingly blurry boundaries among them. In this context, where companies require constant innovation and multidisciplinary skills, those that exclusively make use of their own resources struggle to quickly adapt their products and services to the new environment. Keeping the pace of innovation requires then establishing efficient mechanisms of collaboration with other companies and institutions, both for the generation and filtering of ideas and for the development of the most promising ones. When industry and academic institutions, acting as partners, jointly develop an innovation project, some obstacles usually arise that may stand in the way of achieving its original goals.

This talk deals with some of these possible obstacles as well as strategies for their mitigation, using as an example the collaboration between ITMATI and Repsol in the field of industrial mathematics in their Joint Research Unit in Santiago de Compostela. These examples, though specific to the Oil and Gas sector, may probably be extended to other industrial and service companies.

In the Oil and Gas sector, one of the fastest ways of achieving a competitive advantage goes through the development of methods that allow to perform or improve the simulation, optimization or data analysis of a process, whether this is an industrial process (the operation of technical equipment, the operation of an oil well $\cdots$) or a business process (production planning, investment portfolio planning $\cdots$). In the joint research unit, Repsol pursues a competitive advantage in dealing with different problems of mathematical programming, and tries to obtain that advantage by developing and implementing mathematical and computational methods in sw tools, with immediate application in their business units.

This talk not only discusses different ways of avoiding and mitigating the negative effects of the difficulties that may arise in these joint initiatives, but also how to turn them into opportunities for improvement. Specifically, it deals with how to properly define the goals of the project that are satisfactory for both partners, how to select, balance and dynamically adapt the resources of the project, how and why to keep a strict plan for deliverables but a flexible one for the implementation of mathematical and computational methods, the importance of establishing a common vocabulary among the team, how to keep wide and open communication channels and how to ensure that profitable and transferable results are met.

Keywords: industry, academia, collaboration, research, joint.

Applications of smart data managements and analysis systems in the maritime industry

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Technological advances in data management and analysis together with growing environmental and energy efficiency concerns are creating a new landscape for businesses to operate in. InovaLabs has successfully applied data management techniques in the maritime industries, helping companies and actors in the maritime industries to implement energy efficient and intelligent systems in their day-to-day maritime operations.

Two of these systems are a demand forecast tool for an innovative clean power supply for seagoing vessels at port (related to the GPEC project - Green Port Energy Centre), and an intelligent decision support tool to predict and analyse the impact of energy-efficient and emission reduction measures at port infrastructure (ETAM - Energy Trilemma Advanced Modelling). Both projects are combining mathematical analysis of large quantities of data, and apply these techniques to solve energy efficiency and emission issues of maritime industry players.

The proposed contribution to the conference is a presentation of the two projects described above and describe which problems and necessities of concrete actors in the maritime industry are solved by these systems. The presentation will be a practical illustration of how the systems are applied and which necessities they address.

It is not intended to describe the exact mathematical algorithms of the systems in the contribution to the congress. We understand that such detailed technical mathematics would be handled by other contributions to the conference by participant from academia.

Keywords: Data analysis, Energy Efficiency, Industry 4.0
Acknowledgments.

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Mathematics in the service of emergencies.

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Keywords: Emergencies, LiDAR, geolocation, statistical analysis, safety and efficiency.

INAER is an enterprise of the Babcock group that provides air services, including air services in emergencies such as wildfire, medical emergencies, search and rescue missions, et cetera. A fraction of the missions that INAER performs implies already the use of remote sensors in order to acquire information about the surface of the Earth, be it on shore or off shore. Moreover, right now INAER is bent on expanding the range of services that the company provides, as well as improving the efficiency, quality and safety of present day services. The aim is provide new services and new standards of quality in the current services that will set new standards for the market of aerial services. In order to do so, it is necessary to push the boundaries of the current state of the art of the technology. These changes imply the acquisition of massive amounts of information from a variety of sources, mainly from remote sensors and geolocation services, and combine them with additional spatial data, proprietary and public.

However, acquiring data will not suffice: the cornerstone of the progress forward will be developing the capacity for processing all this data and obtain reliable information, sometimes in real time. In some cases the results will be used for increasing the efficiency, the safety or the quality of the services performed by INAER. In other cases, information products will be delivered directly to the customer in order to assist in decision making processes.

This capacity implies the development and use of algorithms for the systematic process of the data. We can distinguish three main lines of work:

- Process and fusion of spatial data from the surface of the Earth related to properties of the terrain or the surface of the sea. These data may be received via passive or active sensors. Examples of the former are visible spectrum, multispectral and thermal imagery or video. Examples of the latter are radar and LiDAR. This kind of work may be performed in real time or as batch processing. This kind of work is of application in almost all the range of services that INAER provides, from firefighting to search and rescue to land planning, services for the energy sector and more.
- Process of geolocation data in real time. For example, GPS/EGNOS and GSM-obtained position data. Examples of the former are the precise location of aircraft, land resources such as vehicles and troopers, airstrips, watering points, et cetera. Examples of the latter are the positions of GSM devices such as dedicated portable beacons carried by troopers or civilians and mobile phones. This can be used to improve the safety of the troopers and vehicles in emergencies, manage air resources or even search and rescue missions.
- After action, statistical analysis of mission data. This often requires using big data techniques. After action analysis of these huge amounts of data has three main goals:
  - Assessing the safety and efficiency of the missions as they were performed.
  - Improving the safety and the efficiency of future missions.
  - Obtaining answers about phenomena happening on the surface of the Earth that are of interest for the company or directly for the customers. A good example of this would the behaviour of wildfires and the effects of the suppression efforts. Another example would be the assessment of the goodness of supervised classification algorithms, namely, the location of infrastructures using LiDAR data.

MS36: Mathematics behind volcanic processes

MS36: Mathematics behind volcanic processes

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Forecasting the activity of a volcano as a system requires quantitative approaches based on the exploitation of mathematics, physics and computer simulations. This unique combination enables to tackle both theoretical and applied problems in volcanology. Unraveling complex volcanic dynamics and phenomena requires mathematics to provide a universal language that can support drawing and evaluating causal inferences among interacting processes, which accompany the ascent of magma from source to surface, including magma intrusion, hydrothermal activity, conduit flow dynamics, pyroclastic flows and ash dispersal. Volcanology research is strongly interdisciplinary and joint expertise includes nonlinear dynamical systems, statistical data analysis, and numerical modelling. The objective of the minisymposium is to study how volcanological concepts can be formalized using mathematical models and to identify key questions that can be usefully investigated by a cross-view between volcanologist and mathematicians.

Speakers:

Flavio Cannavò. Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Catania (Italy). *Power Laws in Volcanic Systems.*

Elisa Trasatti. Istituto Nazionale di Geofisica e Vulcanologia, Centro Nazionale Terremoti, Rome (Italy). *Volcanic sources retrieved from geodetic data: constraints to their geometry, shape and mechanism.*

María Charco Romero. Instituto de Geociencias, CSIC-UCM (Spain). *Some insights about inversion of volcano deformation based on finite element models: an application to Kilauea volcano, Hawaii.*

Armando Coco. Oxford Brookes University (United Kingdom). *Numerical methods for ground deformation and gravity changes during volcanic unrest.*

In proposing this minisymposium, our motivation is to bring volcanology research toward quantitative approaches enabling the modelling of the involved geophysical processes. Mathematical sciences play a central role in the effort to solve several challenges posed in volcano geophysics both at the modelling and computational level. The interest of ECMI in the mini-symposium is twofold: the models and methods developed in volcanology can be exploited and disseminated in environmental and industrial contexts; the possibility of importing and adopting in volcano research mathematical solutions from other research fields in which similar issues have been already addressed. We aim to attract interest among the applied mathematics community, which could provide interesting new insights and ideas to afford problem in computational volcanology.

Keywords: Computational Volcanology; Mathematical Modelling; Numerical Analysis.

Power laws in volcanic systems

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Volcanoes constitute dissipative systems with many degrees of freedom. Their eruptions are the result of complex processes that involve interacting chemical-physical systems. At present, due to the complexity of involved phenomena and to the lack of precise measurements, both analytical and numerical models are unable to simultaneously include the main processes involved in eruptions thus making forecasts of volcanic dynamics rather unreliable. One characteristic seems to join most of volcanic phenomena, and it is their power-law distribution. In fact, many geophysical processes associated with volcanoes give rise to power-law size distributions, from involved geometries [3] to gas emission rates [1], through volumes of erupted materials [4] and eruption durations [2]. Power-law distributions indicate that besides a large number of small entities the considered process shows a small number, but not as small as expected, of large entities of the same type. Power-law relationships in natural systems are relevant because they have some intriguing features. They are scale free and thus have the same statistical properties at any scale and are not associated with one characteristic scale. In practice, this means that there is no single correct scale for their analysis because the same principles are valid irrespective of the temporal, spatial or strength scale of analysis, and also makes it technically wrong to apply traditional statistics based on variance and standard deviation (such as regression analysis) when dealing with power-law distributed phenomena. The power-law systems share the concept of "universality": it has been shown that completely different systems show similar power-law behaviour on approaching a critical state. Moreover, the indication of a power-law behaviour in some data cannot only explain specific kinds of dynamics that might govern the particular natural phenomenon, but, thanks to the universality, may also indicate a deep connection with other, apparently unrelated systems. While power-law distributions have received great attention in recent decades, the mechanisms behind them are still hardly debated, crossing self-organized criticality process to self-similar stochastic process described by exponential dispersion models. Here we will summarize the evidences of power law hypothesis for different aspects of volcanic systems, highlighting the possible consequences of such an assumption.

Keywords: Power Laws, Eruptions, Volcanic Dynamics.

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Volcanic sources retrieved from geodetic data: constraints to their geometry, shape and mechanism

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Modern Geodesy technologies enable us to measure millimetric surface displacements, to map large and arduous or dangerous areas and to detail elastic/inelastic behaviors from deformation time series in volcanic environments. In turn, mathematical representation of volcanic sources has been improving from very simplified models such as pressurized point-source spheres and opening tensile cracks within a homogeneous half-space to more complicated triaxial ellipsoids arbitrarily oriented in space, moment tensor sources and aggregates of amorphous sources. The main objective is to give insights into the volcanic activity, retrieving the magmatic source parameters (location, depth, shape), and its volume and/or volume variation within inversion frameworks.

In this work we investigate several aspects of the volcanic source retrieval from geodetic data. We consider the common assumption of fixing *a priori* the source shape, discussing the potential bias on the source parameters retrieval. For instance, spherical sources are located shallower than sill-like sources fitting similarly the data. Furthermore, there are cases in which a triaxial ellipsoid, the most general pressurized point-source, may not be suitable, e.g., the recent unrest at Campi Flegrei (2011-2013, 15 cm uplift). In magma intrusion processes across pre-stressed solid rock, a shear stress release takes place, that cannot be provided by pressurized sources. A completely general approach describes a deformation source in terms of a suitable moment tensor distribution and its physical interpretation in terms of a pressurized cavity or else must be proposed only *a posteriori*. We discuss also the effects on the source parameters if the structural heterogeneities of a complex environment such as a volcanic area are taken into account: the source is typically much deeper and the mechanism may differ significantly from homogeneous half-space models. As a final outcome, we inquire the rigorousness of the extension of single source models to amorphous aggregates of small sources, which are suitable to describe thermo-poro-elastic sources, but cannot reproduce pressurized cavities.

Keywords: Physics of Volcanoes, volcano geodesy, numerical modeling, pressurized cavities.
Acknowledgments. This work is partially supported by the MED-SUV Project from the EU's FP7 (Grant Agreement 308665).

Some insights about inversion of volcano deformation based on finite element models : An application to Kilauea volcano, Hawaii

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Geodetic techniques, as Interferometric Synthetic Aperture Radar (InSAR), are being extensively used to monitor ground deformation at volcanic areas. The quantitative interpretation of such surface ground deformation measurements using geodetic data requires both, mathematical modelling to simulate the observed signals and inversion approaches to estimate the magmatic source parameters. In this study, we provide a numerical tool for interpreting deformation measurements by solving the inverse problem to estimate the optimal parameters for magmatic sources in an efficient and accurate way. We propose a Finite Element Model (FEM) for the calculation of Green functions in a mechanically heterogeneous domain. The key aspect of the methodology lies in applying the reciprocity relationship of the Green functions between the station and the source. In our approach, deformation sources are independent of the simulation mesh being incorporated as a source term in the model equations. The search for the best-fitting magmatic (point) source(s) is conducted for an array of 3-D locations extending below a predefined volume region. However, the total number of Green functions is reduced to the number of the observation points by using the, above mentioned, reciprocity relationship. We apply this methodology to the recent inflation episode observed at Kilauea's summit and Southwest Rift Zone in May 2015. We measured the volcano ground displacements using data from the new Sentinel-1 radar interferometry satellite mission. This new methodology is able to accurately represent magmatic processes using physical models capable of simulating volcano deformation in non-uniform material properties distribution domains, which eventually will lead to better description of the status of the volcano.

Keywords: Inverse theory; Finite Element Method; Volcano monitoring
Acknowledgments. This work has been partially supported by the research project CGL2014-58821-C2-1-R.

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Numerical methods for ground deformation and gravity changes during volcanic unrest

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Variations of geophysical parameters in volcanic areas such as ground deformation and gravity changes are usually observed in restless volcanic areas. A correct evaluation of the hazard associated to these signals is fundamental, since they may be indicators of impending eruptions. In particular, it is critical to differentiate the variation of geophysical observables associated with magma migrations from the perturbations caused by the activity of the shallow hydrothermal system. To this purpose, an efficient and accurate numerical model to evaluate ground deformation and the gravity changes associated with hydrothermal activity is presented in this talk. Hydrothermal activity is simulated using TOUGH2, a multiphase multicomponent simulator of fluid flows in porous media. Fluid injection at the base of the system simulates the main unrest period, characterised by fluid of magmatic origins (modelled as a mixture of water and carbon dioxide) that rises from depth. Variations in pressure, temperature and density are evaluated and fed into the thermo-poroelastic and gravity models to evaluate ground deformation and gravity changes. The equations are discretised by a finite-difference ghost-point method in an unbounded domain, in order to avoid artificial boundary conditions.

Although the model is designed for a generic volcanic area, key parameters are based on data available for the Campi Flegrei (CF) caldera (Italy), a volcanic area situated to the west of Naples. In order to simulate a realistic scenario, the model takes into account key complexities that are often ignored, such as heterogeneities in hydrological and mechanical properties and the presence of ring faults.

Since the physics of the hydrothermal system investigated in this talk is similar to any fluid-filled reservoir, the generic model can be employed to monitor and interpret ground deformation and gravity changes induced by a wide range of natural or man-made alterations in the subsurface flows, such as CO2 sequestration and geothermal exploitation.

Keywords: ground deformation, gravity changes, finite difference, unrest simulation, hydrothermal system.

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MS37: Maths for the digital factory

MS37: Maths for the digital factory

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Around one in ten of all enterprises in the EU-27s non-financial business economy were classified to manufacturing in 2009, a total of 2.0 million enterprises. The manufacturing sector employed 31 million persons in 2009, generated 5.812 billion Euro of turnover and 1.400 billion Euro of value added. (source: Eurostat). In the last five or ten years all industrialised countries have launched initiatives related to digital manufacturing, sometimes also referred to as Industry 4.0 (in Europe) or Smart Manufacturing (US).

The minisymposium will provide case studies showing how mathematics will be able to contribute towards digital manufacturing, topics include the coupling of machine, process and workpiece for milling processes, the optimal control of material flow problems on conveyor belts, and the discrete geometric modeling of slender flexible structures for interactive assembly simulation in automotive industry.

Speakers:

M. Pfirsching. Department of Mathematics, University of Mannheim (Germany). *Material flow problems on conveyor belts using a multi-scale model hierarchy.*

A. Schmidt. Center for Industrial Mathematics and MAPEX Center for Materials and Processes, University of Bremen (Germany). *Modelling, simulation, and optimization of thermal distortions from milling processes.*

M. Roller. Institute for Industrial Mathematics, Kaiserslautern (Germany). *Discrete geometric modeling of slender flexible structures for interactive assembly simulation in automotive industry.*

M. A. González. GKN Driveline Vigo, Vigo (Spain). *Numerical simulation of induction heating on ferromagnetic materials parts.*

Keywords: digital manufacturing, industry 4.0, process chains.

Material flow problems on conveyor belts using a multi-scale model hierarchy

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Conveyor belts are used in a wide field of industrial application, for example in bottling plants where a large number of objects is transported at the same time. Here the collision between the material is an intentional part of the transportation process.
As an example problem we study a case where particles move on a conveyor belt as in [1]. One half of the belt is blocked by an obstacle. To compute the movement of the objects hitting the obstacle, we consider two models. The first one is a microscopic model based on ordinary differential equations which calculates a trajectory for each particle with Newton's law of motion as it is described in [2]. The second one is a macroscopic model based on a two dimensional hyperbolic conservation equation with a non local flux function which models the behaviour of the totality of particles (see [1]).
The results of the microscopic model are quite near to real data. But the computation time increases quadratically with the number of particles, so especially for a large number of particles this is not satisfying. Therefore we work with a macroscopic model wherever it is possible. The computation time of the macroscopic model is independent of the mass of particles, but as result one only gets the behaviour of the whole mass, not of each single particle. It turns out that the result of the macroscopic model is quite similar to the result calculated by the microscopic model with a large number of particles. The loss of accuracy is compensated with a decrease of computation time.
Once the problem is simulated, it can be interesting to optimise it, for example to maximise the throughput. In this example problem, the objects should leave the region in front of the obstacle as fast as possible. The control is the placement of the objects on the belt inside a predefined area. The chosen optimisation method is an adjoint calculus combined with a gradient descend method.
By optimising the same setting in both models, it turns out that the optimal solutions for each model are quite comparable, even if the model structure is completely different. The optimisation results for the microscopic model are not satisfying, since there are too many degrees of freedom. In contrast, the optimisation with the macroscopic model provides good results, as well with commercial solvers as with the adjoint method. Finally the optimisation results of the macroscopic model can be interpreted in the microscopic setting. The result is better than any optimisation result one gets by optimising the microscopic model.

Keywords: Particle simulation, conservation laws with non-local flow, optimal control
Acknowledgments. Financially supported by DFG project "OptiFlow".

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Modelling, simulation, and optimization of thermal distortions from milling processes

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The heat produced by a machining process results in thermomechanical distortion of the workpiece and thus an incorrect material removal by the cutting tool. When the resulting deviation from a desired shape is too large, an additional finishing process step is needed. Especially when machining thin walled parts for lightweight structures, the deviations may be quite large. The goal of a process optimization is to minimize the deviation from the desired shape during resp. after the milling process. Thus, the additional process step for corrections can be avoided, the quality of workpieces is improved, and overall speed of production can be increased.

We present a numerical model including the finite element simulation for the thermomechanics, a dexel model for material removal, and a process model for forces and heating produced by the machining tool. This defines the constraints for an optimal control problem. Main control variables are the process parameters and the path of the machining tool. These are varied accorting to the compensation and optimization approach.

The material removal leads to a time-dependent domain, where the most relevant boundary conditions for the thermomechanics are given especially on the moving part of the boundary, where the cutting tool engages. At the same place, deformations lead to incorrect material removal. Thus, good approximations of the time-dependent domain and of the PDE solutions near the moving boundary are important challenges for the simulation and optimization.

Keywords: milling, thermal distortion, finite element method, time dependent domain, optimal control with PDE constraint.

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Discrete geometric modeling of slender flexible structures for interactive assembly simulation in automotive industry

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In industry, there is an increasing demand for using fast (i.e. *real time*) realistic simulation of *slender flexible structures* in software tools for CAD, digital mock-up and virtual assembly, which nowadays can only handle rigid geometries. Typical examples of such structures from automotive industry are cables, tubes and hoses.

For slender one-dimensional deformable objects, the theory of *Cosserat rods* provides a suitable framework for physically correct simulation of deformations like *stretching bending* and *twisting*. The static equilibrium equations of such Cosserat models are given as a set of nonlinear differential equations, which are usually discretized with the Finite Element Method in computational mechanics. This discretization technique provides very accurate simulation results, but is, used in the standard way, computationally far too demanding for fast simulations with an interactive modification of the boundary conditions. The kinematics of Cosserat rods are closely related to the *differential geometry of framed curves*, whereby the strain measures of the rods corresponds to the differential invariants of the curves, like arc length or curvature. Therefore, ideas from the *discrete* differential geometry of framed curves are utilized to construct discrete Cosserat rods. This approach leads to qualitatively correct results, even for very coarse discretizations. Hence, only a small number of degrees of freedom are needed to generate moderately accurate results. This leads to fast computational performance, which makes the discrete Cosserat rod model suitable for interactive simulations.

In our contribution, we present such a geometry based discretization approach for flexible one-dimensional structures, together with some application examples of assembly simulation of cables and hoses in automotive industry.

Keywords: flexible structures, discrete differential geometry, Cosserat rods, fast algorithms.

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Numerical simulation of an induction heating on ferromagnetic materials parts

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The induction hardening is a process based on induction heating and sudden cooling of ferromagnetic materials. This hardening process is a key operation on the manufacturing of a large diversity of parts in the automotive sector. In the case studied, this process is applied to the heat treatment of constant velocity joints to improve the mechanical properties and achieve the required product strength. The numerical solution of a thermo-electromagnetic-metallurgical coupled model allowed us to calculate the electromagnetic fields and the induced currents on the part, the temperature profile along the time and the evolution of the different material phases during the heating cycle.

The benefits associated to the application of this numerical model allowed us the simulation of the hardening case of complex geometries. Moreover, the strategy employed takes into account both the workpiece rotation and the non-axisymmetric character of the inductor without performing three-dimensional simulations which, from the practical point of view, are unaffordable due to their high computational cost. Thus the model let us simulate successive refinements of the inductor design and the corresponding process parameters and, consequently, avoid a large number of empirical trials.

This talk fits in the framework of a collaboration between the company GKN-Vigo with the Research Group in Mathematical Engineering from the Universidade de Santiago de Compostela in order to simulate the industrial problem described above.

Keywords: numerical simulation, induction heating, hardening, thermo-electromagnetic-metallurgical model.

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MS38: Maths in HORIZON 2020 and beyond

MS38: Maths in HORIZON 2020 and beyond

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The MS will discuss opportunities and perspectives of funding Industrial and Applied Mathematics in Horizon 2020. The plan is to have 4 short presentations followed by a round table discussion moderated by Wil Schilders. One presentation is about ECMI and EU-MathsIN, one about successful funding of HPC projects, one about possibilities in production (with a representative from manufuture) and one from a member of EU about their plans to support math in H2020.

Speakers:

V. Alexandrov. ICREA - Barcelona Supercomputing Centre (Spain). *Mathematics and algorithms for extreme scale computing challenges.*

P. Romero. Aimen Technology Centre, Porriño, Pontevedra (Spain). *Factories of the Future in Horizon 2020: Achievements so far and next challenges.*

D. Hömberg. Weierstrass Institute for Applied Analysis and Stochastics, Berlin (Germany). *European collaboration in Industrial and Applied Mathematics.*

A. Hellmann. Deputy Head of Unit Directorate-General for Communications Networks, Content and Technology, European Commission, Brussels (Belgium). *Results of the European Commission's consultation on mathematics for Horizon2020.*

Keywords: HORIZON2020, technology platforms, infrastructures.

Mathematics and algorithms for extreme scale computing challenges

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This talk will focus on the needs for developing novel mathematical methods and algorithms for extreme-scale computing systems and corresponding challenges. The current and emerging extreme-scale systems require novel scientific algorithms to hide network and memory latency, have very high computation/communication overlap, have minimal communication, and have no synchronization points. Scientific algorithms for multi-petaflop and exa-flop systems also need to be fault tolerant and fault resilient, since the probability of faults increases with scale. Also with the advent of heterogeneous compute nodes that employ standard processors as well as GPGPUs, scientific algorithms need to match these architectures to extract the most performance. This includes different system-specific levels of parallelism as well as co-scheduling of computation, etc. Therefore, key science applications require novel mathematics, novel mathematical methods and algorithms as well as system software that address the challenges of current- and future generation extreme-scale HPC systems.

The talk will outline the challenges as well as present the views of ETP4HPC mathematics and algorithms for extreme scale HPC systems working group on possible approaches to address these challenges and needs. Also, with the advent of Big Data in the past few years the need of such scalable mathematical methods and algorithms able to handle data and compute intensive applications at scale becomes even more important. The speaker will present also his views on the novel mathematical methods, algorithms and approaches needed at the interface of Data and Computational Science to address Data and Compute Intensive science placed in the context of the emerging wider research area of Mathematics for Digital Science.

Factories of the Future in Horizon 2020: Achievements so far and next challenges

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In the talk I will recap on the main results of the Factories of the Future research PPP and address main challenges we need to consider towards the second part of H2020. I would also try to highlight, both for the achievements and for the challenges, research topics where mathematics is relevant.

European collaboration in Industrial and Applied Mathematics

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In this presentation I will give an overview of recent activities of the mathematics community for a European collaboration in Industrial and Applied Mathematics. After a short review of mission and interaction of key institutions like ECMI and EU-MATHS-IN, success stories and disappointments in relation to the European Framework Programmes for Research and Innovation will be discussed. I will conclude with some strategic considerations for a fruitful exploitation of industrial and applied mathematics as a key technology for addressing the major challenges in science, technology and society in Europe.

Results of the European Commission's consultation on mathematics for Horizon2020

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Mathematics is recognized today as essential and indispensable for addressing the major challenges in science, technology and society. For example, faced with the abundance of data on social, technical, economic, ecological, and technological systems, new and sophisticated mathematical tools are required for these data to help us tackle pressing societal challenges and provide us with the necessary technological advantages.

In order to understand how mathematics could contribute to the European research, especially in the area of High Performance Computing and Big data analytics, and in general to the development of the Digital Single Market, the European Commission launched an on line consultation on the current mathematical challenges and possibilities. This consultation took place between 28 January and 9 May 2016.

Its aim was to inform the future Horizon2020 work programmes (2018-19-20) with innovative mathematical content, and to look even further beyond – as now is the time to lay the basic foundation for the future research framework programme starting in 2021. It is timely to explore the potential and necessity of mathematics for future research, especially for the areas of high performance computing and data analysis of next generations, and to find ways of bringing that message forward to the prioritization process of the future funding programmes. Two facts motivate this request: today's digital society depends on mathematics and algorithms - and there is a vast pool of mathematical talent in Europe.

The number of contributions was higher than any other consultation we launched simultaneously, thus the consultation was a considerable success.
The purpose of the consultation is further to raise awareness on the latest emerging mathematical areas as well as of the state-of-the-art mathematical solutions and applications, with an ambition of reflecting this in the future Horizon2020 work programmes as appropriate.
The results of the consultation will be distributed widely to the European Commission and shared with the scientific community and all European institutions. They will be available for sharing with the mathematicians.
The preliminary results are already very promising, containing substantive input in areas such as MSO and biomaths, big data analytics and quantum algorithms.
The ECMI conference will be the publication event of the results.

Keywords: Horizon2020, consultation, MSO, biomaths, EC, WP2018-2020.
Acknowledgments. The report bases on the results of the open consultation [1] and contains its main conclusions.

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MS39: Stochastic PDEs and uncertainty quantification with applications in engineering

MS39: Stochastic PDEs and Uncertainty Quantification with Applications in Engineering

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Stochastic partial differential equations are becoming more and more important to model uncertainties, noise, fluctuations, process variations, material properties etc. in various applications.

Stochastic PDEs subsume the usability of PDEs and extend the range of applications that can be modeled. In short, higher-order moments of the solutions can be modeled. The emergence and growth of the field of uncertainty quantification in recent years shows that there is profound interest in these questions in many different application areas.

Modeling and simulation based on stochastic PDEs poses many new and exciting problems regarding the analysis of the solutions, the development of efficient numerical algorithms, optimal-control problems, optimization, and parameter estimation.

This minisymposium brings together researchers in stochastic PDEs and offers an opportunity to discuss the latest developments. Common themes are how uncertain input in engineering problems can be included in mathematical models, how randomness propagates through a PDE model, and how optimization problems can eventually be solved in view of the randomness. Both theoretical aspects such as existence, uniqueness, and regularity of the solutions as well as numerical methods and approaches are covered.

We expect that discussing the similarities of and the differences between leading model equations such as elliptic equations, parabolic equations, the Schrödinger equation, the Boltzmann equation, and the Maxwell equations will be fruitful and provide guidance for future research with applications in engineering.

Speakers:

Jianyu Li, Roger Ghanem. Tianjin University of Science and Technology, Tianjin, China; University of Southern California. *Numerical solution method for stochastic variational inequalities with polynomial chaos decompositions..*

José A. Morales Escalante, Irene Gamba. ICES, UT Austin. *Reflective boundary conditions in discontinuous Galerkin methods for Boltzmann-Poisson models of electron transport in semiconductors and zero flux condition for general mixed reflection..*

Marc Dambrine, Charles Dapogny, Helmut Harbrecht. Universität Basel. *Shape optimization for quadratic functional and states with random right-hand sides..*

Zeger Bontinck, Oliver Lass, Sebastian Schöps. TU Darmstadt. *Robust optimization of the size of permanent magnets in a synchronous machine using deterministic and stochastic approaches..*

P. Benner, Akwuzm Onwunta, M. Stoll. *Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg. Fast solvers for optimal control problems constrained by PDEs with uncertain inputs..*

Numerical solution method for stochastic variational inequalities with polynomial chaos decompositions

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We build on the product space nature of the polynomial chaos decomposition to extend the standard variational inequality constructions to functional spaces adapted to the stochastic case, which has wide range of applications in describing the problems with interfaces, contact, plasticity, and phase transformation that exhibit variability in material properties. We describe mathematical and computational challenges and demonstrate the formalism by taking example of plasticity problems in mechanics. A random projection algorithm will be proposed to solve the stochastic variational inequalities with polynomial chaos decompositions and some numerical results will be presented.

Keywords: Stochastic Variational Inequalities, Polynomial Chaos Decompositions, Projection Algorithm, Plasticity.
Acknowledgments. Partially supported by the National Natural Science Foundation of China (No. 11272234).

Reflective boundary conditions in discontinuous Galerkin methods for Boltzmann - Poisson Models of electron transport in semiconductors & zero flux condition for general mixed reflection

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We shall discuss the use of Discontinuous Galerkin (DG) Finite Element Methods (FEM) to solve Boltzmann - Poisson (BP) models of electron transport in semiconductor devices at nano scales. We consider the mathematical and numerical modeling of Reflective Boundary Conditions in 2D devices and their implementation in DG-BP schemes. We derive analytical and numerical relations that satisfy a net zero flux of mass across physical boundaries in which specular, diffusive or mixed reflection BC occur, by means of a balance between the inflow and outflow of electron transport at these boundaries. We study numerically these specular, diffusive and mixed reflection BC on physical boundaries of the device for the modeling of surface roughness, comparing the influence of these different reflection cases in the computational prediction of moments close to the boundaries and their associated scale. We observe an effect due to diffusivity at the reflection boundaries over the kinetic moments of the probability density function, whose influence is not restricted to the boundaries but rather over the position space domain.

Keywords: DG, Transport, Semiconductors, Reflection, Boundary Conditions, Boltzmann - Poisson
Acknowledgments. Supported by ICES & Math Department at The University of Texas at Austin.

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Shape optimization for quadratic functionals and states with random right-hand sides

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In this talk, we investigate a particular class of shape optimization problems under uncertainties on the input parameters. More precisely, we are interested in the minimization of the expectation of a quadratic objective in a situation where the state function depends linearly on a random input parameter. This framework covers important objectives such as tracking-type functionals for elliptic second order partial differential equations and the compliance in linear elasticity. We show that the robust objective and its gradient are completely and explicitly determined by low-order moments of the random input. We then derive a cheap, deterministic algorithm to minimize this objective and present model cases in structural optimization.

Keywords: shape optimization, random right-hand side, quadratic functional.

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Robust optimization of the size of permanent magnets in a synchronous machine using deterministic and stochastic approaches

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The goal of this work is to reduce the size of the buried permanent magnets (PMs) in a PM synchronous machine. Since the machine is modeled in 2D, only the width and the height of the magnets are changed. The magnet is also allowed to be repositioned deeper into the rotor or closer to the surface of the rotor. While changing these parameters, a prediscribed electromotive force (EMF) has to be maintained.

In a nominal optimization one looks for the miminal size of the magnets. However, due to mass production, small deviations on the dimensions of the PMs can occur, i.e., the found optimum could become sub-optimal. To consider these deviations two approaches can be used. The first one is robust optimization, where the worst case deviation is considered. By doing this, one takes the sensitivity of the minimum into account. The second approach is a stochastic approach, where the deviations are modelled by random variables and their distributions are taken into account.

The local sensitivities can be determined by the derivatives of the EMF. For the global sensitivity, which is used in the stochastic setting, one uses statistical moments (e.g. standard deviation). These values are obtained by using stochastic collocation. The relation between robust and stochastic optimzation are investigated mathematically and by using a numerical example.

The electrical machine is modeled using the magnetostatic formulation of Maxwell's equations. Once the field quantities have been determined using the finite element method (e.g. [1]), one can calculate the EMF by the loading method [2]. To decrease the computational cost, model order reduction (the Reduced Basis Method) and an affine decomposition [3] is applied to a region around the PM.

The approaches are able to reduce the amount of PM material while maintaining the predescribed EMF.

Keywords: Finite element analysis, Monte Carlo methods, permanent magnet machines, Optimization.
Acknowledgments. This work is supported by the German BMBF in the context of the SIMUROM project (grant nr. 05M2013), by the 'Excellence Initiative' of the German Federal and State Governments and the Graduate School of CE at TU Darmstadt.

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Fast solvers for optimal control problems constrained by PDEs with uncertain inputs

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Optimization problems constrained by deterministic steady-state partial differential equations (PDEs) are computationally challenging. This is even more so if the constraints are deterministic unsteady PDEs since one would then need to solve a system of PDEs coupled globally in time and space, and time-stepping methods quickly reach their limitations due to the enormous demand for storage [4]. Yet, more challenging than the afore-mentioned are problems constrained by unsteady PDEs involving (countably many) parametric or uncertain inputs. This class of problems often leads to prohibitively high dimensional saddle-point system with Kronecker product structure, especially when discretized with the stochastic Galerkin finite element method (SGFEM) [3]. Moreover, a typical model for an optimal control problem with stochastic inputs (SOCP) will usually be used for the quantification of the statistics of the system response – a task that could in turn result in additional enormous computational expense.

In this talk, we consider two prototypical model SOCPs and discretize them with SGFEM. We derive and analyze robust Schur complement-based block diagonal preconditioners for solving the resulting stochastic Galerkin systems with all-at-once low-rank solvers . The developed solvers are quite efficient in the reduction of temporal and storage requirements of the high-dimensional linear systems [2, 1]. Finally, we illustrate the effectiveness of our solvers with numerical experiments.

Keywords: Stochastic Galerkin system, iterative methods, PDE-constrained optimization, saddle-point system, low-rank solution, preconditioning, Schur complement.

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MS40: Computational methods for finance and energy markets

MS40: Computational methods for finance and energy markets

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This MiniSymposium is an activity of the ECMI Special Interest Group on Computational Finance [2]. The SIG was launched at ECMI-2014 in Taormina (June 9-13, 2014) and (together with the ITN STRIKE network [3]) organized several sessions of a minisymposium in Computational Finance. The corresponding reporting can be found in [1]. At ECMI-2016 we bring together again twelve speakers.

The computational complexity of mathematical models employed in financial mathematics has witnessed a tremendous growth. Advanced numerical techniques are imperative for the most present-day applications in financial industry. The aim of this MiniSymposium is to present most recent developments of effective and robust numerical schemes for solving linear and nonlinear problems arising from the mathematical theory of pricing financial derivatives and related financial products.
These approaches vary in departing directly from the system of stochastic differential equations (involving SABR dynamics) to approaches for the derived partial differential equations. The SDE group focusses on fast Monte-Carlo methods involving COS methods and techniques for GPU processors. The PDE group discusses efficient finite difference methods (varying in involving techniques like sparse time integrators by alternating direction methods, or boundary element methods), also combined with pseudospectral methods. Further speakers will discuss concisely aspects like Credit Value Adjustment, Counterparty Credit Risk and effects due to uncertainty in parameters.

In the recent years we observe an increasing interest in mathematical methods for energy markets as well. The rapid changes in energy trading within the last two decades have attracted many researchers in academia and industry. Their aim is to adequately model energy prices and typically also to design methods and guidelines for risk management challenges. Existing modelling tools and numerical methods for this application field face several new kinds of challenges.
Coupled with highly inelastic demand and a variety of supply side constraints, the lack of energy storage can result in sudden price spikes and high, time-varying volatility. Mean reversion rates and typical seasonal patterns exhibit a complex multi-scale nature with respect to the time variable. Calibration is an essential ingredient to obtain realistic models. The models need to have a detailed specification with the various quantiles being related to multiple factors through coefficients which have dynamic properties themselves related to some of the exogenous factors.

Speakers:

Álvaro Leitao, TU Delft and CWI-Amsterdam (the Netherlands): *On an efficient one and multiple time-step Monte Carlo simulation of the SABR model*.

Qiang Feng, CWI-Amsterdam (the Netherlands): *Credit Value Adjustment, Wrong Way Risk and Bermudan Options*.

Mark Cummins, DCU Business School, Dublin City University (Ireland): *Model Risk in Gas Storage Valuation: Joint Calibration-Estimation Risk Measurement*.

María Suárez-Taboada, Universidade da Coruña, A Coruña (Spain): *Uncertainty Quantification and Heston model*.

Andreas Binder, MathConsult GmbH, Linz (Austria): *Developing a tool-chain for computational finance in a regulated universe*.

Zaza van der Have, TU Delft and CWI-Amsterdam (the Netherlands): *The COS method for option valuation under the SABR dynamics*.

Michael Schürle, University of St. Gallen (Switzerland): *Optimization of hydro storage systems and indifference pricing of power contracts*.

Florentina Paraschiv, University of St. Gallen (Switzerland): *Estimation and application of fully parametric multifactor quantile regression with dynamic coefficients*.

Jose G. López-Salas, Universidade da Coruña, A Coruña (Spain): *Parallel stratified regression Monte-Carlo scheme for BSDEs with applications in finance*.

Christian Hendricks, Bergische Universität Wuppertal (Germany): *Hybrid finite difference / pseudospectral methods for stochastic volatility models*.

Michael Günther, Bergische Universität Wuppertal (Germany): *Stochastic volatility models calibration with Model Order Reduction*.

María del Carmen Calvo-Garrido, Universidade da Coruña, A Coruña (Spain): *PDE modeling and numerical methods for swing option pricing in electricity markets*.

Keywords: computational finance, energy markets, energy trading, energy risk management, option pricing, barrier options, SABR, calibration, tool development, credit risk, power contracts, quantile regression, pseudospectral methods, uncertainty quantification, BSDEs, stochastic grid bundling method, price spikes, time-varying volatility, seasonal patterns, multi-scale models

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On an efficient one and multiple time-step Monte Carlo simulation of the SABR model

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In the works [3] and [4], we propose an efficient Monte Carlo simulation for the SABR model [2]. The technique is based on an efficient simulation of SABR's integrated variance process. The integrated variance process appears in the SABR model simulation since it is part of the conditional cumulative distribution of the SABR forward asset dynamics.

We base our approach on the derivation of the cumulative distribution function of the integrated variance and the use of a copulas to approximate the conditional distribution (integrated variance conditional on the SABR volatility process). For that, a recursive procedure based on the COS method [1] is employed here. This Fourier-based methodology recovers the probability density function given the corresponding characteristic function. Several improvements in terms of efficiency are proposed.

Different types of copulas are compared like Gaussian, Student $\mathbf{t}$ and Archimedean copulas. In order to determine the most suitable one, a *goodness-of-fit* analysis of each one is carried out.

Resulting is a fast and accurate simulation algorithm. The one time-step version can be employed to price European options under the SABR dynamics. This converts this approach into an alternative to Hagan analytic formula for short maturities and calibration procedures, where some known issues of the implied volatility expression for small strike values are overcome. On the other hand, the multiple time-step extension of our technique is specially useful for long-term options and for exotic options.

We present a variety of experiments where the accuracy and the performance of our method is shown.

Keywords: SABR model, Monte Carlo simulation, Integrated variance, Copula.
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Credit value adjustement, wrong way risk and Bermudan options

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Credit value adjustment (CVA) is an capital charge introduced in Basel III to improve the bank's resilience against future loss due to the default of the counterparty. The complexity of computing CVA arises from the uncertainties of the losses of a default event (exposure), the likelihood of the counterparty's default in the future (default probability), and the implicit dependence structure between exposure and default probability. When the counterparty's credit quality and the associated exposure is adversely correlated, the effect called wrong way risk (WWR) incurs. Banks are required to identify and monitor WWR in Basel III as this effect may make significant contribution to CVA.

Bermudan option holders have the right to exercise the options in a set of time steps, and thus may change the early exercise strategy when they want to reduce the counterparty credit risk (CCR). Banks will be overcharged if they compute CVA of Bermudan options without considering the changed behaviors of the option investors in a default circumstance.

This paper proposes an affine model to describe the dependence structure between the underlying equity and the default probability of the counterparty based on intensity approach. By defining concepts of default-free and default-adjusted values, we present that CVA values that accounts WWR or RWR in the future time steps can be computed without nest Monte Carlo simulation under this framework, which enhances the computational efficiency greatly.

In this paper we show that the Monte Carlo method SGBM (Stochastic Grid Bundling Method) and the Fourier cosine expansion method COS can both be applied efficiently to price Bermudan options in this context. We analyze the impact of CCR and WWR on Bermudan options. We compare the optimal early exercise values obtained with two types of exercise principles: one is aimed to maximize the default-free value, and the other is to maximize the default-adjusted value. The results show that a risk-averse option holder will exercise the option earlier when there is more likelihood of a default event. We further see that the CVA of a Bermudan option is smaller but not eliminated when it is exercised by maximizing the default-adjusted value. The optimal early exercise values are also different when WWR or RWR incurs.

Keywords: CVA, WWR, Bermudan option, Monte Carlo, Fourier cosine expansion, COS, SGBM
Acknowledgments. Financial support by the Dutch Technology Foundation STW (project 12214) is gratefully acknowledged.

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Model risk in gas storage valuation: joint calibration-estimation risk measurement

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We present a joint calibration-estimation risk measurement methodology, extending recent literature, which incorporates *both* market calibration and historical estimation risk within a meaningful distributional assessment of parameter risk. Extending the emerging literature on model risk issues in energy markets, we apply our technique to the problem of natural gas storage valuation, using a flexible multi-factor Mean Reverting Variance Gamma model specification that is *both* forward curve consistent and calibrated to market traded options. Realistic models of the natural gas forward curve cannot be calibrated to benchmark instruments alone due to the lack of a liquid time-spread options market and thus the correlation structure is typically estimated from historical data. We additionally devise an accessible model selection technique based on our distributional assessment of parameter risk. For a basic one-year $20in/20out$ storage contract, we show that the parameter risk of our two-factor Mean Reverting Variance Gamma model is higher relative to single-factor Mean Reverting Variance Gamma and Mean Reverting Jump-Diffusion benchmarks, with very different distributional characteristics. Formally pricing the parameter risk, shows the model based bid-ask spread to be over five times that of the benchmarks. The greater flexibility of the two-factor Mean Reverting Variance Gamma model in capturing more extrinsic value therefore comes at the cost of greater uncertainty. Our novel model selection technique shows, however, this increased uncertainty to be bearable, concluding that the two-factor Mean Reverting Variance Gamma model is an acceptable choice over its one-factor counterpart.

Keywords: model risk; parameter risk; gas storage models

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Uncertainty quantification and Heston model

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In general, stochastic differential equations governing the prices of certain financial products do not always have an analytical solution. The required numerical approximations used do not contain enough information about the reliability of the output of a certain mathematical model and randomness can be present in different inputs which introduces uncertainty into the solution of the model. These issues make mathematical models in computational finance a good framework to apply Uncertainty Quantification (UQ).

The so-called volatility smile appears in many financial markets, as an important feature of pricing models. Among the sophisticated models developed to reproduce it, the Heston model ([3]) has become one of the most used for practitioners and it will be the focus of this work.

Heston model describes the dynamics of the stock price and the variance where a set of parameters is considered which can be seen as stochastic and providing randomness and uncertainty to the model. Despite being many other sources of uncertainty, we are concerned here with uncertainty in model parameters and focus on the propagation of the uncertainty from them to the output. The Stochastic Collocation Method already used in computational fluid dynamics, has been applied to compute such propagation ([1] [4]). Main objective is to compute the probability distribution and the statistical moments of the output of interest when the response surface is approximated locally by a polynomial function. We could see that the propagation of the uncertainty is dominated by the computational cost of the numerical solver. Due to this, it is important to choose an efficient numerical method with a low computational cost as the COS-method ([2]).

Firstly, Heston model and UQ framework are introduced. Then, numerical examples with Feller condition satisfied and not are presented to show the good performance of the method. As a first approach, only two parameters have been considered, obtaining a 2-dimensional problem for UQ. Next, the whole set of parameters is taken from real market data dealing with a 5-dimensional problem. Finally, some conclusions about the impact of the variability of the parameters are presented.

Keywords: Uncertainty Quantification, Heston Model, Implied Volatility, COS-Method.
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Developing a tool-chain for computational finance in a regulated universe

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After the breakdown of Lehman Brothers and after the financial crisis of several member states of the European union, computational finance has significantly changed its face: Up to 2007, new emissions of financial instruments tended to be quite complex and often exhibited features like multiple underlyings, path dependence and/or multiple callability. We now observe financial instruments which can be valuated with fairly simple tools, at least in a risk-neutral environment.

However, the concept of risk-neutrality is no longer valid, even not for simple Libor instruments. In so-called multicurve models, different interest rate curves have to be used for forwarding and discounting, increasing the dimensionality of the describing (partial or stochastic) differential equations.

Under the Basel III regulation, banks are required to calculate the market value of counterparty credit risk for every counterparty on their balance sheet. The value of this (unilateral) credit valuation adjustment (CVA) depends on the credit quality of the counterparty and of the distribution of future cash-flows depending on future market developments. The calculation of such CVAs may become extremely computationally challenging as even fairly simple positions may require to perform millions of valuations for each instrument in the exposed portfolio.

Regulation is not only applied in the bank-to-bank environment but also to bank-to-customer relationships. When advising a customer, banks (or other financial advisers) have to obey the regulation on key information documents for packaged retail and insurance-based investment products (PRIIPs) and the markets in Financial Instruments Directive (MiFID, to be followed by MiFID 2). Advisers have to check the knowledge and experience and the risk profile of the investors. A clear presentation of risks, an appropriate analysis of scenarios and stress tests, and a thorough documentation of the advisory process is essential for future success.

We present recent results from the views of mathematical algorithms and of efficient data management, obtained within the UnRisk environment.

Keywords: Computational Finance.
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The COS method for option valuation under the SABR dynamics

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Efficient valuation of financial derivatives is an important issue in financial mathematics. Fourier methods, such as the COS method [1, 2], employ the characteristic function of the underlying asset process to determine the option value, where a characteristic function is the Fourier transform of the underlying density. However, often no analytic expression for the characteristic function of the underlying process is available, like for the SABR model.

This model, also known as the "stochastic alpha beta rho model", is since the introduction of the Hagan formula [3] in 2002 a widely used stochastic volatility model. We propose to use the bivariate characteristic function of the discretized SABR process to price European and Bermudan options, where we use the Euler-Maruyama or the 2.0-weak-Taylor scheme for the discretization. The application of these schemes in combination with the COS method results respectively in first-order and second-order convergence.

Second-order convergence can also be obtained by using Richardson extrapolation in combination with an Euler-Maruyama discretization on the forward process, which provides a significant reduction in computational costs compared to the 2.0-weak-Taylor scheme.

We also solve backward stochastic differential equations by using the discretized stochastic processes and the Fourier-cosine expansion. For this purpose we use the BCOS method (Backward Stochastic Differential Equation COS method) [4], which we extended from one to two dimensions.

Keywords: COS method, BCOS method, Euler-Maruyama scheme, backward stochastic differential equation, SABR, Richardson extrapolation, option pricing.

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Optimization of hydro storage systems and indifference pricing of power contracts

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In this paper, we aim at a mid-term planning model for hydropower production based on multistage stochastic optimization. We decide about a production schedule for a horizon of one year from the point of view of a producer that owns pumped-storage hydropower plants. These consist of large seasonal connected reservoirs. We consider stochastic inflows, stochastic electricity prices and stochastic loads. The optimization of hydropower production is based on multistage stochastic programming with an aggregation using price levels to overcome the curse of dimensionality. The produced electricity is sold at the spot market. In addition, we follow an indifference pricing approach for non-standard power contracts to determine the price at which the producer is willing to deliver electricity to individual consumers.

The dynamics of electricity prices is described by a novel regime-switching approach where a base regime is distinguished from two spike regimes that reflect large price movements down- or upwards. A price is considered to be in one of the spike regimes if it is below or above some limit values which will be estimated simultaneously with the other model parameters. This allows for a more realistic fit to the data than the common approach in the literature where regime limits are set to three standard deviations.

We analyze historical data for the inflows in each reservoir from an existing system in the Swiss Alps. The inflows in each reservoir will be simulated jointly based on two driving factors that are identified by principal component analysis. The generated scenarios will be aggregated to a scenario tree using scenario reduction techniques. In each node of the scenario tree we will have information about the possible price levels for electricity in the upcoming week and about the level of inflows. Based on this information, we decide about generating, pumping or overflows at different price levels. These decisions will be updated in weekly steps.

Our objective is a mixture of expectation and average value of risk over the revenues at the end of the planning horizon of one year.

In addition to the model for power dispatch optimization, we formulate a second multistage stochastic programming model to determine the price at which the producer is indifferent with respect to selling the produced electricity on the spot market or entering in individual power contracts. We take into account as well individual demand profiles of consumers. The indifference price is computed for different levels of risk aversion.

To our knowledge, this is the first study in the literature which proposes indifference pricing for multiple contracts in the context of hydropower and it is of particular relevance for the risk management and production planning of power plants holders.

Keywords: Multistage stochastic programming, scenario aggregation, hydropower dispatch, indifference pricing
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Estimation and application of fully parametric multifactor quantile regression with dynamic coefficients

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This paper develops and applies a novel estimation procedure for quantile regressions with time-varying coefficients based on a fully parametric, multifactor specification. The algorithm recursively filters the multifactor dynamic coefficients with a Kalman filter and parameters are estimated by maximum likelihood. The likelihood function is built on the Skewed-Laplace assumption. In order to eliminate the non-differentiability of the likelihood function, it is reformulated into a non-linear optimisation problem with constraints. A relaxed problem is obtained by moving the constraints into the objective, which is then solved numerically with the Augmented Lagrangian Method. In the context of an application to electricity prices, the results show the importance of modelling the time-varying features and the explicit multi-factor representation of the latent coefficients is consistent with an intuitive understanding of the complex price formation processes involving fundamentals, policy instruments and participant conduct.

We demonstrated the value of a well specified dynamic model for quantile estimation by means of an application to electricity price risk. Electricity prices are a commodity in which price formation is nonlinear in its relationship to fundamentals, dynamic in the relative influences of drivers, with further complications introduced by policy interventions for supporting specific technologies and opportunities for participant conduct to be influential at high and low prices. Despite these complications careful consideration of the shape of the supply function with its concave, flat and convex regions, together with the information that is available to market participants day ahead allows plausible expectations for the price dynamics to be considered, and these explain very well the signs and significance of the parameters in the estimated models. Nevertheless, the models need to have a detailed specification with the various quantiles being related to multiple factors through coefficients which have dynamic properties themselves related to some of the exogenous factors. This modelling requirement motivates the development of quantile models that need fully parametric specifications to capture dynamics through exogenous factors and time-varying coefficients.

Keywords: Quantile Regression, Dynamic Coefficients, Parametric Estimation, Electricity Prices
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Parallel stratified regression Monte-Carlo scheme for BSDEs with applications in finance

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In this work we design a novel algorithm based on Least-Squares Monte Carlo (LSMC) in order to approximate the (Y, Z) components of the solution to the decoupled forward-backward stochastic differential equation (BSDE)

$$Y_t = g(X_T) + \int_t^T f(s, X_s, Y_s, Z_s)\mathrm{d}s - \int_t^T Z_s \mathrm{d}W_s,$$
$$X_t = x + \int_0^t b(s, X_s)\mathrm{d}s + \int_0^t \sigma(s, X_s)\mathrm{d}W_s,$$

where W is a $q \geq 1$ dimensional Brownian motion. The algorithm will also approximate the solution to the related semilinear, parabolic partial differential equation.

In recent times, there has been an increasing interest to have algorithms which work efficiently when the dimension d of the space occupied by the process X is large. This interest has been principally driven by the mathematical finance community, where nonlinear valuation rules are becoming increasingly important. Currently available algorithms [1, 2, 3, 4] rarely handle the case of dimension greater than 8. The main constraint is not only due to the computational time, but mainly due to memory consumption requirements by the algorithms.

The purpose of this paper is to drastically rework the algorithm of [4] to first minimize the exposure to the memory due to the storage of simulations. This will allow computation in larger dimension d. Secondly, in this way the algorithm can be implemented in parallel on GPU processors which enables us to obtain substantial speedups compared to CPU implementations. We present several numerical examples in order to illustrate the performance of the scheme. For further details, see [5].

Keywords: Backward stochastic differential equations, dynamic programming equation, empirical regressions, parallel computing, GPUs, CUDA.

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Hybrid finite difference / pseudospectral methods for stochastic volatility models

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In this work we propose a hybrid spatial finite difference / pseudospectral discretization for partial differential equations (PDEs) of stochastic volatility models. As a testbed for two factor models we consider the Heston PDE [2] and the Heston-Hull-White equation [3] functions as a testbed for three factor models.

The initial condition of option pricing problems is in general non-smooth: for example in the case of digital options the payoff itself exhibits a discontinuity at the strike price whereas for European options the first derivative of the payoff suffers from a discontinuity. This non-smooth nature of option pricing problems makes it difficult to design numerical schemes, which achieve a high rate of accuracy in practice. Thus, we propose a hybrid discretization, which employs a standard second order finite difference discretization in direction of the underlying asset, where the non-smoothness occurs, while we use a Chebyshev collocation method in direction of the volatility and interest rate. In the time domain we employ alternating direction implicit schemes [1, 4] to efficiently decompose the system matrix into simpler one dimensional problems. This approach allows to compute numerical solutions in a multi-dimensional setting, which are second order accurate in time and asset direction and exhibit spectral accuracy in the other spatial domains.

In numerical experiments we evaluate the stability properties as well as the accuracy of the hybrid method. In the time domain we observe an unconditional stable behavior in all test scenarios. In space the geometric error decay of the spectral approximation allows to use significantly less grid nodes compared to a pure second order finite difference discretization. Thus, the hybrid scheme is able to outperform its benchmark method in terms of achieved accuracy versus run-time.

Keywords: stochastic volatility models, Heston model, Heston-Hull-White model, spectral method, finite difference method, alternating direction implicit scheme.

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Stochastic volatility models calibration with Model Order Reduction

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This work presents the calibration of a stochastic volatility model, the Heston Model, using Model Order Reduction [1]. The calibration within the context of financial markets usually goes along the following lines: after choosing a suitable model or models to the behaviour of the particular market, e.g. FX Markets, Stock Markets, etc., the information regarding currently priced instruments in the market is gathered. Using simple, quick models one obtains an estimate of at which value of the parameters is the market currently trading. These estimates are posteriorly used to priced more complex/exotic products.

A very simple calibration process involves a least-squares minimization problem in which each cost function evaluation involves solving one partial differential equation (PDE) per each set of parameters available on the market. This can quickly become prohibitively expensive to solve numerically. For that reason two parallel strategies are presented in this work, which should improve considerably the cost of such calibrations. Two approaches to solve option pricing PDEs are usually available: the forward and the backward ones, where the advantages of one in comparison with the other is related with the number of parameters of the model, as well as the output of interest.

On the first approach, the backward equation one, we start with a terminal condition (payoff function) at the expiration date (maturity), solve it backwards in time until the present time and obtain the price for the derivative for different values of the current spot-price. However, the data available in the market comes from prices for different strikes and maturities. If we are interested in the prices for different strike prices, we solve the PDE with a different terminal condition. If we are interested in the prices for different maturities, we solve the PDE with a terminal condition at a different time.

On the second approach, the forward equation one, we fix the trading day information, i.e., the spot-price and the current date, and solve forwards the adjoint PDE, which will give us the spot-price conditional density distribution for different spot-prices and times in the future. To obtain the derivative price we calculate the expectation of the payoff and discount it to the present time (or other time of interest).

Applying model order reduction to these two models allows us to improve the efficiency of this procedure, as the models still depend on parameters, e.g., the interest-rate r, the volatility σ, the dividend rate q, etc. and we need a quick and accurate enough model to calibrate some of these parameters which are not directly observable in the market.

Obtaining reduced versions of the above mentioned models, we proceed to calibrate option prices to market data by the above mentioned least-squares minimization. We present the results showing the computational efficiency and comparing it with the ones resulting from a parametric reduced order model. We use alternating-direction implicit (ADI) schemes to numerically solve the PDEs in both approaches.

Keywords: computational finance, stochastic volatility model, Heston model, calibration, model order reduction, adjoint PDE, Alternating-Direction Implicit time integration

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PDE modeling and numerical methods for swing option pricing in electricity markets

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After liberalization of electricity markets, prices are stated from the supply and demand principle, thus increasing volatility and uncertainty. So, companies use contracts to protect themselves from high prices and take advantage from low prices. Swing options represent a standard contract and mainly consist of path dependent options giving the holder the right to exercise certain right multiple times over a period, including the constraint that two consecutive exercises must be separated by a refracting period. Swing options pricing gives rise to interesting mathematical and numerical problems. Binomial trees, Monte Carlo methods and partial differential equations (PDEs) for one stochastic factor have been used in the literature. Following [6], in this work we consider two stochastic underlying factors describing the electricity price dynamics. According to [7], the swing pricing can be posed as a sequence of free boundary problems, one per each exercise right. Since, the obstacle function associated with the free boundary problem involves the contract value with one exercise right less, additionally an initial boundary value problem has to be solved.

In order to solve the pricing problem, we propose appropriate numerical methods based on a Lagrange-Galerkin discretization of the involved PDE problems [1, 2], combined with the augmented Lagrangian active set method, proposed in [5], to cope with the free boundary problems. Moreover, by using the ideas in [4], we derive appropriate artificial boundary conditions to be applied to the localized bounded domain obtained from the initial unbounded one. Finally, some numerical results are presented in order to illustrate the performance of the numerical schemes and the observed properties of the solution. More details can be found in [3].

Keywords: swing options, electricity price, option pricing, complementarity problem, Augmented Lagrangian Active Set formulation, Lagrange-Galerkin discretization, artificial boundary conditions.
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Contributed talks

CT01: Finances

Computation of market risk measures with stochastic liquidity horizon

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The Basel Committee of Banking Supervision (BCBS) states in recent consultative documents that the financial crisis exposed material weaknesses in the overall design of the framework for capitalising trading activities. Due to that, a review of the trading book regime was initiated. Among others, the BCBS has focused on incorporating the risk of market illiquidity as a key consideration in banks' regulatory capital requirements for trading portfolios. During the crisis, banks were forced to hold risk positions for much longer than expected and incurred in large losses. The most important risk metric in banking for the last 20 years has been the Value-at-Risk (VaR), but a number of weaknesses were identified such as its inability to capture the risk in the tail of the profit and loss distribution. For this reason, the expected shortfall (ES) was introduced, which is the expected value of all changes in the portfolio value conditional on these changes exceeding the VaR.

All this above motivates our research work. Some studies suggest that liquidity risk could be addressed by extending the risk measurement horizon. Our purpose is to present a set of numerical techniques to compute the VaR and ES risk measures under a stochastic liquidity horizon. This idea was first introduced by [1] and we give a step further by considering different dynamics to drive the portfolio like the delta-gamma approach or by well known dynamics on the log-returns such as GBM, Merton jump-diffusion or KOU models.

To evaluate risk measures, Monte Carlo simulation is often used, but obtaining accurate estimates is computationally expensive. Here we adopt scenarios where the characteristic function of a fixed portfolio change is known in closed form. We provide a procedure to express the characteristic function of a stochastic time horizon portfolio change from the deterministic one. Fourier techniques to invert this characteristic function in a market risk context can be applied. We employ an approach based on wavelets. Specifically, we provide methodology for computing the VaR and ES using SWIFT. The SWIFT (Shannon Wavelet Inverse Fourier Technique) method [2] is based on a Shannon wavelet expansion of an underlying density function for pricing European options. Shannon wavelets are smooth wavelets based on the cardinal sine function. From its nature SWIFT presents several benefits such as high accuracy, robustness, fast convergence, the density approximation does not deteriorate with the choice of the domain size, the number of terms needed are automatically calculated, FFT can be applied to enhance speed and estimation of the error is available. Because of that, we use SWIFT to approximate the portfolio change density function.

Concluding, we present formulae for computing a portfolio VaR and ES with a stochastic liquidity horizon by approximating the portfolio change density by a Shannon wavelet expansion. That procedure gives a robust method with accurate results which face the impact of the market illiquidity.

Keywords: Liquidity risk, Stochastic liquidity horizon, VaR, ES, Fourier Transform, SWIFT.
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A Fourier-wavelet based dimension reduction method for option pricing

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We present a robust and highly efficient Fourier-wavelet based dimension reduction method for computing plain-vanilla European option prices and hedging parameters under general jump-diffusion models with stochastic variance and multi-factor Gaussian interest rates. Using the conditional Monte Carlo technique applied to the variance factor, the option price can be expressed as a two-level nested conditional expectation. The inner expectation is then evaluated analytically, with the variances associated with all the interest rates factors completely removed from the analytical solution. The outer expectation is approximated very efficiently by means of the Shannon Wavelets Inverse Fourier Technique (SWIFT) via evaluating a single integral that involves only the variance factor. Central to this process is a highly efficient recovery of the conditional density of the time-integrated variance process using the SWIFT method. Furthermore, the SWIFT method also allows us to develop sharp approximation error bounds for the option price and hedging parameters. Numerical experiments confirm the error bounds, robustness and efficiency of the proposed pricing method.

Keywords: Shannon wavelets, Fourier inversion, dimension reduction, jump diffusion, stochastic volatility.

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CT02: Fluid structure interaction

Numerical simulation of flow induced vocal folds vibration by stabilized finite element method

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This paper is interested in the numerical simulation of human vocal folds vibration induced by fluid flow, see [1] or [2]. A general problem of fluid-structure interaction is formulated. An attention is paid to the description of a robust method based on finite element method. In order to capture flow velocities involved in the physical model, the modified Streamline-Upwind/Petrov-Galerkin (SUPG) stabilization is applied, for example [3].

The first part contains mathematical description of problem, where the arbitrary Lagrangian-Euler method (ALE) is used to solve the fluid flow on time dependent domain. The viscous incompressible fluid flow and linear elasticity models are considered. In the second part the numerical scheme is described for the fluid flow and the elastic body and the implementation of coupling between them is explained. The numerical results are shown.

Keywords: Stabilized finite element method, 2D Navier-Stokes equations, vocal folds, aeroelasticity.

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The riser system motion reconstruction

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The marine riser system undergo different types of loadings: vertical tension, loading from surface waves and fluid current, loading from ship movement. These lead to the periodic riser motion and may become cause of riser equipment failure due to fatigue. That's why it is important to control riser motion. High interest of oil industry in the qualitative motion reconstruction confirms actuality of the problem. The main goal of this work is to receive motion reconstruction based on data from few sensors installed through the length of the riser system as well as to calculate curvature and stress field. Reconstruction method is based on Fourier decomposition of true riser shape. Dynamic FEM of riser system is used to compare the quality of reconstruction.

Keywords: motion reconstruction, marine riser, VIV.
Acknowledgments. The work is supported by "FMC Technologies".

CFD simulation of river Viv

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Riser system for deep water applications are subjected to various type of loading. One of the phenomena's the installation may experience during the lifetime is so called VIV. This type of vibration may occur when the frequency of the structure matches the vortex shedding frequencies. Hence, the monitoring of structures is of high concern. Therefore it is urgent to take measurements to mitigate and prevent fatigue failures or potential riser failures resulting from VIV fatigue.

The main goal of this work is to develop fluid structure interaction model (FSI) of the submerged riser system and a reliable mathematical model that simulates two ways coupling between CFD and Structural codes, it also implies evaluation of coupling method and parameters between CFD and Structural codes.

Keywords: VIV, FSI, CFD, riser.
Acknowledgments. The work is supported by "FMC Technologies".

CT03: Applications of data analysis and statistical methods

GPS positioning and long baselines processing

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Networks RTK are now common in Europe. However, this is not the case in emerging economies where huge construction projects are running requiring geodetic support. In such cases, the easiest way to ensure that kind of support still is the static relative positioning using a single reference station. This technique provides surveyors the ability to determine the 3D coordinates of a new point with centimeter-level accuracy relative to a control point located several hundred kilometers away, which in turn can be associated with another GNSS receiver of a Continuously Operating Reference Stations (CORS) operated by some institution. The objective of this research is to evaluate GPS static relative positioning [2, 3, 4], regarding accuracy, as the equivalent of a network RTK and to address the practicality of using either a CORS or a passive control point for providing accurate positioning control. The precision of an observed 3D relative position between two GNSS antennas, and how it depends on the distance between these antennas and on the duration of the observing session, was studied. This goal was achieved by comparing the outputs from the Leica Geo Office v5 (LGO) software and the Ordnance Survey (OS) active stations coordinates, assumed as true. The methodology followed was using observation files from OS active stations to simulate different scenarios for the baseline length, in order to answer the question of how long should be the observing session for the LGO to process those baselines within a pre-establish threshold of accuracy. A descriptive approach can be found in [6]; also different statistical techniques, namely data analysis and elementary/intermediate inference level [5] and general linear models [7] were successfully applied. An extention of such approach is presented in this work, where a more complete multivariate analysis [1], adequate methods to analyze the kind of data in study, is still going on.

Keywords: GPS, Long Base Lines, Data Analysis, Multivariate Analysis
Acknowledgments. This work was supported by Portuguese funds through the *Center for Computational and Stochastic Mathematics* (CEMAT), *The Portuguese Foundation for Science and Technology* (FCT), University of Lisbon, Portugal, project UID/Multi/04621/2013, and *Center of Naval Research* (CINAV), Portuguese Naval Academy, Portuguese Navy, Portugal.

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A methodology for fasteners placement to reduce a gap between the parts of the wing

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The process of airplane's wing assembly is known to be very complex and demanding in terms of precision. It is necessary that during this process a gap between fastening parts be small. Otherwise, critical stresses may appear causing damage to the wing. The main problem addressed in our study is to develop methodology of fasteners placement, so that it is suitable for several wings at once. Due to uncontrollable factors, different wings have deviations in form, so the gap between the parts of the wing will be varying as well. In this case, it is natural to use a stochastic approach and model the gap as a random field, then our goal will be to reduce this gap to a certain level with given probability by specific positioning of the fixing fasteners.

One of the issues that come to the fore in our study is that one of random field parameters estimation as it is hard to get sufficient amount of reliable measurements. In this case we are bounded to use small samples statistics methods instead of the classic ones. These methods come in handy as a last resort choice when there are no other options available.

Results of our study were implemented as an algorithm that produces sequence of positions to place fasteners into. In future, our approach may be useful in some other closely related problems as well.

Keywords: wing assembly, fastening process, random field, small samples.

Using hypothesis testing in order to evaluate improvement actions implemented in the production process of a metallic component for the automotive industry

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Quality measurement and control is an activity that has a high level of importance throughout the supply chain in the automotive industry. This work was developed in collaboration with a second-tier supplier of various automotive manufacturers that produces, among other products, car seats. The process analysed was the one where the metallic frame of a rear backrest for an automobile is produced. One of the issues studied was the process capability measured by the indices C*p* and C*pk*, which connect the specification limits imposed by the client or by the development team, to the real variability of the process, measured by its standard deviation [1], [2].

The indices C*p* and C*pk* are extensively used in the automotive industry and for numerous characteristics of the products. In this work, 9 safety characteristics of the referred metallic frame were studied and it was found that one of them did not meet the minimum values of C*p* and C*pk* established defined by the company. The process was then analysed and improved in order to increase the process capability related to that characteristic [3]. Given that the observed values of the characteristic presented an approximately normal distribution (the test K-S Lillefors was performed on the data and the null hypothesis was not rejected), the tests on the variance ratio (test F) and on the means difference (test t) before and after the implemented improvements were performed [4].

It was found that, with a level of significance of 5%, the variances of the characteristic decreased and the mean changed towards a more centered value regarding the specification limits. It was then possible to conclude that changes made to the process resulted in real improvements on the safety characteristic analysed and, consequently, on the respective capability indices.

Finally, it is considered that the outcomes of this work are valuable not only for researchers on industrial data analysis applied to the quality area, but also for the industry staff in general, that can use the proposed methodology in other environments.

Keywords: Quality Control; Process improvement; Process Capability; Hypothesis Testing.
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SMED applied to the setup of a glazing operation: tests of hypothesis to evaluate mean setup times and variance reduction

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The increase of competiveness has led companies to embrace the principles and tools of Lean Manufacturing as a way of reducing waste and thus becoming more capable of facing the challenges the present-day market presents. One of those tools is SMED (Single Minute Exchange of Die) that is used to reduce setup times for equipment or workstations [1]. The origin of SMED can be associated with the origin of the Toyota Production System since it was developed by Shigeo Shingo at the Toyota Motor Company [2]. The use of SMED can help reduce setup times (which are considered waste) but also increase flexibility, since lower setup times allow for more product changes and smaller production batches, thus helping the production system respond more quickly to changes in demand. The impact of the use of SMED in setup times can be evaluated using statistical techniques to find out if that reduction is indeed significantly relevant and, moreover, if the variance of those times also was reduced thus indicating a more organized and stable setup process.

This work was developed at a company that produces stoneware tableware. One of the stages of the production process is the glazing of the parts and changes in colour and/or part require a setup operation of the glazing cabins. The setup times for that operation, before the use of SMED, were registered considering, for this analysis, eight situations (representative of the three identified categories of setups), and then 20 observations for each one were collected. Due to time constraints regarding the duration of the work only two of those situations (the more complex ones) were analysed after the implementation of SMED. With the data from those two situations, K-S tests were performed and it was possible to consider that the setup times (before and after SMED) presented an approximately normal distribution. Finally, hypothesis testing to compare the mean setup times (t tests) and variance (Bonett's test) were applied [3].

It was found that, with a level of significance of 5%, both the means and variances of the setup times decreased. This led to the conclusion that the implementation of SMED principles induced a reduction of setup times, and the standardization of the setup tasks helped to decrease their variability. This study can be an important contribution for researchers on industrial data analysis but also for practitioners that wish to implement SMED (or other lean techniques) and evaluate their impact in the reduction of waste.

Keywords: Lean Manufacturing; SMED; setup reduction; hypothesis tests.

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Control charts for monitoring an obstetrician service performance

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Control and improvements of the quality of hospital services are of crucial importance since they are a public health subject. In the recent decades, public healthcare organizations have turned their attention to the continuous monitoring quality of the provided services employing performance metrics as answer times of labs, post-operative recuperation days, waiting times, patient satisfaction scores, medication errors, emergency service response times, infection rates, mortality rates, numbers of patient falls, among many others.

Although there are often clear clinical indications for a cesarean delivery, the short and long-term benefits and risks for both, mother and infant, have been the subject of intense debate. Cesarean delivery involves major abdominal surgery and is associated with higher rates of surgical complications and maternal rehospitalization, as well as with complications requiring neonatal intensive care unit admission. In addition to health and safety risks for mothers and newborns, hospital charges for a cesarean delivery are almost double of those for a vaginal delivery, imposing significant costs. Therefore, the percentage of cesarean deliveries is a widely used indicator of quality performance in hospital obstetric services. High values of cesarean rates may indicate that a significant percentage of the cesarean deliveries have no clinical reason and there are external factors, as social or cultural ideologies, organizational management, physician practice patterns, among others, acting on the process.

In this work the evolution of the rate of cesarean deliveries in a public Portuguese healthcare organization is analysed, using control charts for statistical control process. The data was collected during the year of 2014 and the first semester of 2015 obtaining a mean value of cesarean rates of 26.65% with a standard deviation of 5.15%. This value is better than the last Portuguese average value in 2012 (35,9%) but worst than the World Health Organization (WHO) recommended value (15%). Several control charts, with different sample sizes, were designed in order to analyse suspicious variations and therefore, the presence of external factors affecting the process. Considering weekly and monthly samples, the rates of cesarean fall between the corresponding control limits. On the other hand, when daily samples are considered, there are one value falling on the upper control limit and only two values falling outside it. These last results may indicate the presence of external factors, and therefore a non-stable process, the α-risk is also higher since the sample size is smaller. In this way, a special attention should be given to the process, implementing weekly control charts and EWMA or CUSUM charts, to detect small variations in the process mean which may result in a quality deterioration.

Keywords: control charts, statistical process control, obstetrician performance.

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CT04: Numerical simulation of batteries

Thin-film electrodes for high-capacity lithium-ion batteries: Influence of phase transformations on stress

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Based on recent work that show a two-phase process of lithiation of amorphous silicon, we formulate a phase-field model coupled to elasticity in the framework of Larché-Cahn. Using an adaptive nonlinear multigrid algorithm for the finite-volume discretization of this model, our two-dimensional numerical simulations show the formation of a sharp phase boundary between the lithiated and the amorphous silicon that continues to move as a front through the thin layer. We show that our model captures the non-monotone stress loading curve and rate dependence, as observed in recent experiments and connects characteristic features of the curve with the stucture formation within the layer. We take advantage of the thin film geometry and study the corresponding one-dimensional model to establish the dependence on the material parameters and obtain a comprehensive picture of the behaviour of the system.

Keywords: Phase Separation; Li-ion Batteries; Strain Energy; Asymptotics; Phase-Field Modelling

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Numerical simulation of a Li-ion cell using a thermoelectrochemical model including degradation

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A thermoelectrochemical model for the simulation of Li-ion cells is presented herein. The model, based on Newman's [1] concentrated-solution theory, covers electrochemical, thermal and aging effects. The degradation mechanism considered is the growth, due to a solvent decomposition reaction, of the Solid Electrolyte Interface layer, SEI, on the graphite anode. Model homogenization is phenomenological but detailed particle-scale models are considered for the diffusion of species within active particles and SEI.

The model is posed on a one-dimensional domain, consisting of three subdomains, where temperature, solid phase potential and electrolyte phase variables are solved, coupled with three two-dimensional problems for solving solid phase concentrations for the different species. The one dimensional thermal model incorporates the reversible, irreversible, and ohmic heats generation, as well as the temperature dependence of the various transport, kinetic and mass-transfer parameters based on Arrhenius expressions.

The nonlinear governing equations are discretized using the finite element method with Lagrange P1 elements and implicit Euler in time, and solved fully coupled with a Newton method. The solver has been developed by using FEniCS software package [5].

Numerical results and comparison with experimental data on the literature will be presented.

Keywords: Li-ion batteries, Butler-Volmer, thermoelectrochemical, aging, numerical simulation, mathematical modeling.

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Numerical simulation of a network of Li-ion cells using a thermoelectrochemical model

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The battery system of an electric vehicle comprises hundreds of battery packs connected in both parallel and series, plus many other electric components required for the correct charge, power and thermal management of the system. Furthermore, each battery pack is a stack of several individual electrochemical cells connected in parallel and thermally coupled.

The aim of the present work is the numerical simulation of a pack of Li-ion cells. To this end, the device is modeled by an RCL circuit whose unknowns are $I_k, k \in \{1, \ldots, N_b\}$, the currents on the N_b branches and $V_k, k \in \{1, \ldots, N_p\}$, the potentials at the N_p nodes. On the branches containing a cell, a model based on Newman's [1] concentrated-solution theory that covers electrochemical, thermal and aging effects is considered. The cells are coupled through Kirchoff current law [2] and (eventually) thermal effects. The algebraic-differential system is discretized using an implicit finite difference scheme.

More precisely, when computing the unknowns at time step n, the constitutive law on a branch with a cell is given by

$$I_k^n = \mathrm{DtoN}(v_k^n) \qquad \text{or} \qquad v_k^n = \mathrm{NtoD}(I_k^n)$$

where v_k^n is the voltage on branch k at time step n (the difference between the potentials at both ends of the branch) and the operator $\mathrm{DtoN}(v_k^n)$ (resp. $\mathrm{NtoD}(I_k^n)$) provides the current (resp. the voltage) by solving the cell model for the corresponding datum. At each time step the non-linear system with $N_b + N_p$ equations is solved using Newton's method. The performance of this iterative procedure with respect to the operators that are used on each cell ($\mathrm{NtoD}(\cdot)$ or $\mathrm{DtoN}(\cdot)$) is carefully analyzed.

Since on each Newton's iteration, the resolution of the electrochemical cells is completely decoupled, they can be solved in parallel leading to a computationally efficient algorithm. When a thermal coupling between cells is considered, a weak coupling between the macroscopic temperature of the device and the individual thermal contributions of each cell is performed allowing to preserve the efficiency of the global discretization procedure.

Keywords: Li-ion batteries, electrical networks, numerical simulation, stack of cells, electric vehicle.

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CT05: Optimization problems

Optimization of conveyor system loading

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In this work, optimization of throughput of belt conveyor systems for transportation of bulk material in mine industry is under consideration. The continuous mining systems consist of load and haulage equipment (underground loader and/or dumper), feeder-breaker (scraper conveyor with crusher), local or side (chamber block) belt conveyor and main belt conveyor [1, 2]. Belt conveyor systems with long distance and huge traffic are the main delivery equipment in mines. Open conveyor systems have material entry and exit points and materials go across the system only once. The main purpose is to introduce optimal control algorithm for loading of such conveyor systems to improve the performance efficiency, and avoid possible overloading of the main underground conveyor. The length of this is about 3 kilometres, changing according to the underground working face advance and it has technical boundaries for load capacity. If these are overrun, the whole system stops automatically. Removing the overload is practically possible only manually, this takes lot of time and will result in significant economic damage. The objective of control is to maximise the output of the whole conveyor system versus given initial constraints and to avoid the load amounts which exceed the allowed technical parameters. This is possible through the improvement of control of loading operation at feeder-breaker and means the computing of appropriate downloading instants for dumpers or loaders. Arriving of loaders is random and the information about the loader is transmitted to the central server by RFID system. The volumes of underground loaders are up to 14 tons and dumpers are up to 20 tons and for technical reasons the filling process of side conveyors has to be quite slow. E.g., for output from feeder-breaker filled by dumpers or loaders the content of 9-ton bucket, about 80 seconds are foreseen. Computing the unloading times or, the same - waiting times for loader drivers is the main possibility to avoid overloading of the main conveyor. Mention that different unloading points can have different productivity; the time for the same loader can vary by unloading points. Described problem of conveyor system loading control has no linear programming solution because of its discrete/continuous nature. In this work, we replace real conveyor system with virtual system of conveyors and spatial domain is replaced with time domain [2]. Main control and computing criteria are achieving optimal efficiency of the whole system, avoiding overloading of the system and minimizing waiting times of loaders. Loading permissions for loader drivers are computed on the base of fist-in-first-out queuing. Described approach for control of conveyor system loading process is implemented in Estonian mining company VKG [3]. We discuss the results of this implementation in the presentation.

Keywords: queue modelling, conveyor system, operation efficiency, loading control, spatial and time domain.
Acknowledgments. Partially supported by institutional research funding IUT20-57 of the Estonian Ministry of Education and Research, and VKG AS.

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A heuristic method to optimize high-dimensional expensive problems - application to the dynamic optimization of a WWTP

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The models describing many industrial processes often consist in a large number of algebraic-differential equations. The numerical simulation of such models in standard workstations may lead to high computation times (from minutes to hours). Performing optimization tasks with these models results in unaffordable computation times, thus, there is a need of optimization methods that reduce the number of simulations to locate optimal solutions [1]. The use of surrogate model-based algorithms, and in particular kriging and radial basis functions, has been subject of study by several authors in different disciplines [2]. They can be defined as statistical interpolation/prediction methods which make use of a surrogate model to estimate the location of the optimal solution in the real model. One of the main drawbacks of these methods is that the overhead associated to building the surrogate models increases with the problem dimension and with the number of simulations performed. Since many problems in engineering optimization and design are high dimensional, the applicability of these methods is limited. Even if recent advances have been made in the field of large-scale expensive optimization [3], it is still a subject under research. In this work we propose a heuristic method based on an evolutionary algorithm to optimize computationally expensive high dimensional problems. The algorithm analyzes the information provided by the real simulations and is guided by a set of selected solutions and different indexes designed to account for quality and diversity. Preliminary tests show that this method is not as much affected by the problem dimension as other popular methods like kriging, providing high quality solutions in a low number of simulations compared to other optimization methods.

The algorithm has been successfully tested using a realistic model of a waste water treatment plant [4] to carry out the dynamic optimization of two control variables: aeration and recycle flow rate. Using the control vector parameterization approach a 40 variable problem has been formulated. The proposed method is able to locate the best known solution in shorter computation times than traditional and surrogate-based optimization methods.

Keywords: computationally expensive models, dynamic optimization, heuristics, evolutionary algorithms, WWTP.
Acknowledgments. This research has received financial support from the Spanish MINECO (and the ERDF) through the projects referenced as DPI2011-28112-C04-03, DPI2011-28112-C04-04, DPI2014-55276-C5-2-R, AGL2013-48993-C2-1-R and the grant BES-2014-070946.

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A second order fixed domain approach to a shape optimization problem

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A fixed second order domain approach for solving optimal shape design problems is presented. The original optimal shape design problem is converted to an optimal control problem defined on a fixed domain. First and second order optimality conditions are derived. Numerical results are presented which demonstrate the robustness of the second order method.

Keywords: Shape optimization, Optimal control, Penalization, Newton method.
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Wing section optimization for yacht design via multiresolution methods.

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The equilibrium of a sailing yacht is defined by the balance between the force on the sails (aerodynamic) and the righting moment (weight) and also the force on the hull and appendages (hydrodynamic). Appendages: like keel which is used to provide lift to counter the lateral force from the sails or rudder which is used to steer the boat are designed like plane wings: with a plan form (global shape) and sections (2d aerodynamic profile). So part of appendages efficiency (enhance boat performance) depends on their sections: the quantity of lift and drag they generate in function of fluid characteristics and speed. Each appendage has specific characteristics: structural requirement, plan form area, etc and to optimize a section we take into account those parameters and find an optimum section shape in function of the lift and drag we want.

We consider this problem from the standpoint of signal processing, using multi-scale techniques. More precisely, using subdivision schemes for the generation of curves, we have decomposed the section of an appendage into several detail scales. The search of the optimum shape with this treatment is easily implemented and can be executed very fast.

We present results for 2D implementations which provide good expectations about the extension to real 3D yacht components.

Keywords: Optimization, yacht design, sections, multiresolution methods.

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Design of tensegrity structures by using real code genetic algorithms.

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In this paper we apply genetic algorithms to find the optimum design of a tensegrity structure. Tensegrity structures consist of a set of cables, which are working under tension and a set of struts, which only work under compression. The concept of tensegrity has been applied to sculptures, but it can be also found in several architecture and civil engineering proposals because of it leads to light, robust and elegant designs. The process of determining the shapes and self-stress states of tensegrity structures leads to an optimization problem involving several variables hard to manage. Genetic Algorithms are a type of Evolutionary Algorithms for optimization based on the principles of natural selection and genetics. They have been proven to be useful in several structural optimization problems and particularly in some phases of the form-finding process of tensegrity structures. Usually, genetic algorithms are complementary tools to get, for example, a set of force densities that guarantee a required rank deficiency matrix. We propose a different strategy that consist on applying genetic algorithms to find the optimum design of a tensegrity structure regardless minimum mass or deflection from a global and comprehensible point of view. The whole structure is parameterized and the algorithm deals with the problem without extra knowledge of it. An efficient real codification is considered and the appropriate operators selected. The adequate selection of parameters, operators and parallelization of the algorithm provide minimum mass or deflection structures.

Keywords: Optimization, Evolutionary Algorithms, Tensegrity, Structures.
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Sequencing industrial cutting patterns with interval graphs

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Industrial cutting operations involve taking large objects of standard sizes (stock material such as wooden panels, paper rolls, aluminum profiles, flat glass) and cutting them into smaller pieces of different sizes to meet customers' demands. A *cutting pattern* is defined by specifying how many small items of each size will be cut from each large panel and where the cuts will be made. Typical cutting stock problems deal with the generation of a set of cutting patterns that minimizes waste. But, beyond pattern generation, the issue of defining the sequence in which the patterns are cut can be of importance. The *Pattern Sequencing Problems* consist in finding the permutation of the predetermined cutting patterns that optimizes a given objective function.

The *Minimization of Open Stacks Problem* (MOSP) is a pattern sequencing problem that appears in flat glass, paper, and wood cutting industries. If a cutting machine processes just one cutting pattern at a time, the items of the same type already cut are piled in a stack by the machine, which remains near the machine if there are more items of that type to be cut in a forthcoming pattern. A stack is closed and removed from the working area only after all items of that type have been cut. After a pattern is completely cut and before any stack is removed, the number of open stacks is counted. Because of space limitations around the cutting machines, and other reasons, it is advantageous to minimize the number of open stacks, and that can be done by finding an optimal sequence to process the cutting patterns [3]. The *Minimization of Order Spread Problem* (MORP) arises when it is desirable to keep all the pieces cut belonging to one order as close in time as possible, as, for instance, in the glass cutting industry, where the glass pieces have to be handled and stored individually. Reducing the time elapsed between cutting all the pieces corresponding to the same order cuts down the handling and storing costs.The *Minimization of Discontinuities Problem* (MDP) consists in finding a cutting pattern sequence such that the number of discontinuities is minimum. A *discontinuity* occurs when an item that is being cut in a given pattern is not cut in the following pattern and is cut again later. The difference from MORP is that the duration of the discontinuities does not influence the cost of the solution, just its existence.

In this talk we present an integer programming model, based on the edge completion of a MOSP graph and on a characterization of interval graphs that uses a perfect elimination ordering of the vertices [1]. Although these pattern sequencing problems are NP-hard problems that are not equivalent to the MOSP, and not even to each other [2], their solutions have a similar structure. The concepts related to interval graphs, comparability graphs and chordal graphs, can provide insight to the structural properties of the admissible solutions of Pattern Sequencing Problems. MOSP models may also be combined with cutting stock models to tackle the integrated cutting stock and pattern sequencing problem.

Keywords: Minimization of Open Stacks Problem, Pattern Sequencing Problems, Cutting stock, Integer Programming, Graph Layout, Interval Graphs.

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Optimization and sensitivity analysis of trajectories for autonomous small celestial body operations

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The number of space missions designed for the investigation of small celestial bodies is increasing. They provide the opportunity to obtain detailed knowledge about the composition of asteroids and thereby to learn more about the evolution of our solar system as well as to find rare earth elements. Such deep space missions require autonomous spacecraft systems due to the large spatial distances and mission times. To realize on-board calculations of orbit maneuvers, high precision methods of non-linear optimization and optimal control can be used.

We present corresponding infinite-dimensional optimal control problems and their transformation into finite-dimensional non-linear optimization problems via a direct discretization method. For this transcription a multiple shooting method is chosen, providing high accuracy in solving the dynamic models. The resulting high dimensional problems are solved by the NLP solver "WORHP", which provides high precision methods of non-linear optimization using sequential quadratic programming and interior point methods. Furthermore, within the problem formulation the competitive mission aims short flight time and low energy consumption can be weighted.

Subsequently, a parametric sensitivity analysis for certain perturbation parameters of state and control variables is implemented. Perturbations are, e.g., deviations in parameters like the specific impulse of the spacecraft or the chosen weighting factor of the mission aim. These may have a great impact on the practicability of a planned trajectory. The parametric sensitivity analysis is on-board capable and gives an approximation of the perturbed optimal trajectory as well as the perturbed optimal control. This way, it allows for a stability analysis of the optimal solution while only the nominal solution needs to be evaluated.

For the evaluation of our approach, orbit maneuvers are investigated considering different priorities of energy cost and flight time. Parametric sensitivities of different optimization variables are analyzed and their impact on the nominal trajectories is discussed. The results presented demonstrate the enrichment for autonomous decision making regarding orbit maneuvers by providing a range of trajectories including stability information. In addition, the application of the developed algorithms in the fields of autonomous driving and deep sea navigation is discussed.

Keywords: guidance, multiple shooting method, non-linear optimization, optimal control, sensitivity analysis, trajectory planning.
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Optimal shape design for polymer spin packs

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Polymer spin packs are widely used for the production of synthetic fibers and nonwoven materials. The influence of heat within the spin pack can cause polymer degeneration and therefore it is essential to keep the overall residence time as short as possible. We apply mathematical shape optimization for the design of spin pack cavities with a low and homogeneous residence time. Our design goal in terms of a cost function is to minimize the distance between the wall shear stress and a given target wall shear stress across the surface of the cavity. This enables us to design shapes with a sufficiently high wall shear stress and thus without any stagnation zones where polymer degeneration can take place.

In our talk we cover the whole range from the theoretical background, over the numerical treatment of the shape optimization problem and up to real world applications with our industrial partners. We begin by studying the controllability of linearized shape-dependent operators to classify the space of reachable wall shear stresses. We present our numerical approach for solving the shape optimization problem and show how to deal with certain regularity issues. Finally, we close our talk with applications and demonstrate how mathematical shape design was successfully applied to improve industrial polymer spin packs.

Keywords: Shape Optimization, Controllability, Partial Differential Equation
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Numerical methods for optimization problems: an application to energetic districts

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The electric system has been experiencing a dramatic evolution in the last years, mainly drove by the massive spread of renewable energies and by the increasing attention to energy efficiency and emission reduction. A much smarter electricity system is required, in which each customer would be able to support system stability by means of active load response, as well as by using generators and energy storage systems that may be localised at their premises.

Within this framework, Enel Research and Innovation has developed a software package to optimize the energy resources management of industrial districts, with the aim of minimizing the customer energy bill, [2]. Taking into account real time information on customer energy needs and production, and forecasts on energy requirements and availability at customer, and on energy market prices in the next hours, a cost function is built that should be minimized.

Here we focus on the solution of the arising constrained optimization problem. We describe the two solvers that have been employed for its solution: a Sequential Linear Programming, [3] and a Particle Swarm Optimization, [1], [4]. The performance of the two solvers is compared on realistic models of industrial districts and on a real district. It is shown that the use of the package would allow savings in the energy bill, with respect to the standard paradigm in which energy is produced when required by loads, [5].

Keywords: Particle Swarm Optimization, Sequential Linear Programming, constrained nonlinear optimization, energy management.

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Modeling and optimization applied to the design of fast hydrodynamic focusing microfluidic mixer for protein folding.

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In this work, we are interested in the design of a microfluidic mixer based on hydrodynamic focusing which is used to initiate the folding process (i.e., changes of the molecular structure) of a protein by diluting a protein solution to decrease its denaturant concentration to a given value in a short time interval we refer to as mixing time. Our objective is to optimize this mixer by choosing suitable shape and flow conditions in order to minimize its mixing time [1]. To this end, we first introduce a numerical model that enables computation of the mixing time of a considered mixer. To reduce the computational time needed to solve our design problem, this model is implemented in both full three-dimensional (3D) and simplified two-dimensional (2D) versions; and we analyze the ability of the 2D model to approximate the mixing time predicted by the 3D model. Then, we define a mixer optimization problem and solve it using a hybrid global optimization algorithm. We verify the robustness of the optimized result by performing a sensitivity analysis of its parameters [2]. We achieve a design with a predicted mixing time of 0.10 μs, approximately one order of magnitude faster than previous mixers [3].

Keywords: Microfluidic mixers; Shape design; Numerical Modeling; Global Optimization; Sensitivity analysis.
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Galerkin method using optimized wavelet-Gaussian mixed bases for electronic structure calculations in quantum chemistry

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Many applications of quantum chemistry involve *ab initio* simulations. These are feasible thanks to well-known approximations to the Schrödinger equation, such as Hartree-Fock's or density functional theory [1]. More than 70 softwares are available to chemists in this field, the most common ones being VASP, Gaussian and ABINIT. A key difference between them lies in the basis functions selected to express the molecular orbitals. One of the newcomers, the massively parallel program BigDFT [2], uses wavelet bases for performance considerations.

To better capture the cusp singularities of the orbitals in the *all-electron* calculations without increasing the complexity of BigDFT, we suggest enriching the wavelet basis by Gaussian functions $g_{I,q}(x) \sim \exp(-|x-X_I|^2/2\sigma_{I,q}^2)$ centered at each nucleus position X_I. The unknown orbitals are then approximated by linear combinations $\phi(x) = \sum_{I,q} \alpha_{I,q} g_{I,q}(x) + \sum_k \beta_k \chi_k(x)$ where χ_k denote the scaling/wavelet functions.

To optimize the construction of additional Gaussian functions, we rely on a combination of *a posteriori* error estimates and the greedy algorithm. We adapt the ideas from [3] to establish that the dual norm of the residue can serve as an effective estimate for the energy decrease between the pure-wavelet solution and the augmented-basis solution. Furthermore, in a similar spirit with reduced-basis techniques [4], we recommend the greedy algorithm for building an incremental sequence of additional Gaussian functions.

As a proof of concept to this strategy, we investigate a one-dimensional model of Schrödinger type with delta potentials, which represents a system of one electron and M nuclei of known charges and positions. Due to the small number of additional degrees of freedom, wavelet-Gaussian mixed bases exhibit a significant gain in accuracy while having a low computational cost. It testifies to the interest of this approach.

Keywords: molecular simulation, Galerkin method, Gaussian, wavelet, mixed basis, error estimate.

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Applying metaheuristics algorithm for distribution of monitoring stations in pollution area

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The environmental issue of air pollution is one of the very important issues in modern society. Countries develop various strategies for monitoring and measuring the level of air pollution. Despite good plans, sometimes it is not possible to realize such strategies because of the limitations such as variability of conditions in the measurement area, rapid climate changes or lack of funds. Thus there is often a need to adapt those strategies to real life conditions using different optimisation methods. In this paper we present the usage of the metaheuristics algorithm Variable Neighbourhood Search (VNS) to determine optimal geolocations of monitoring stations through optimisation. VNS has been successfully applied in combinatorial optimisation and global optimisation for problems such as location theory, cluster analysis, scheduling, vehicle routing, artificial intelligence, or engineering. We will also give a visual interpretation of the solution using Geographic Information System (GIS) technology. Integration of results within a GIS system and overlaying monitoring stations geolocations with other spatial layers can improve crosscheck, supervision and comprehension.

According to a document published by the Ministry of Agriculture and Environmental Protection, of the Republic of Serbia, a clear strategy for monitoring and measuring air pollution in Serbia was defined. However, despite a larger number envisaged by the strategy only 27 monitoring stations could have been realized on the territory of Belgrade which covers the area of $3222km^2$ and has a population of 1576124 within 166 settlements. Positioning of monitoring stations can be based on different conditions. In this paper we propose an optimisation approach based on the criterion of the number of population covered by monitoring stations. Namely, we will define the positions of 27 monitoring stations in the 166 settlements in such way that the largest number of population is covered. The mathematical definition of problem is to find: $max\{f(x)|x \in X, X \subseteq S\}$ where S is the solution space, X is the feasible set, x is a feasible solution, and $f(x)$ is the real-value objective function. From the mathematical point of view this problem might not look complex, as one can try all possible distributions of monitoring stations, calculate the population covered, and at the end choose the combination of monitoring stations which covers the largest population. But there are $\binom{n}{k} = \binom{166}{27} = 8.599156876874483 \cdot 10^{+30}$ ways of distributing the stations, which makes calculation and comparison of all distributions practically impossible. Our solution for this problem is based on the VNS algorithm, which starts from a possible solution and explores its distant neighbourhoods, moving to a new solution if and only if an improvement is made. Automatisation of this solution enables adaptations of the algorithm to different conditions, such as different coordinate systems, different radius of measurement instruments, different number of stations and the like.

Keywords: VNS, air pollution, optimisation, max.

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CT06: Homogenization and asymptotic methods

A variational approach to the homogenization of a variable exponent power law magnetostatic problem

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In materials science is crucial to give a macroscopic description of composites with a periodic microstructure made off materials with different properties. The mathematical theory of homogenization focuses on the asymptotic analysis of boundary value problems which describe microscopically the behaviour of such heterogeneous media. We are interested in describing the asymptotic behaviour of the magnetic permeability of a composite made off alternate layers of different materials and characterized by a nonlinear constitutive power-law relation. We consider the variational formulation of the stationary Maxwell equations in Magnetism supplemented by a variable exponent power-law constitutive relation and assuming that the composite has a perfectly conducting boundary.

Keywords: stationary Maxwell equations, effective properties, composite.
Acknowledgments. Partially supported by the research project MTM2013-47053-P from MINECO.

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Convergence of equilibria of thin inextensible von Kármán rods

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We study the effects of simultaneous homogenization and dimension reduction in the context of convergence of stationary points for thin inextensible non-homogeneous rods under the assumption of the von Karman scaling. Given $\Omega = (0, L) \times \omega \subset \mathbb{R}^3$ a three-dimensional rod-like canonical domain of length $L > 0$ and cross-section $\omega \subset \mathbb{R}^2$, the (scaled) energy functional of a rod of thickness $h > 0$ associated to a deformation $y^h : \Omega \to \mathbb{R}^3$ is defined by

$$\mathcal{E}^h(y^h) = \int_\Omega W^h(x, \nabla_h y^h)\mathrm{d}x - \int_\Omega f^h \cdot y^h \mathrm{d}x\,. \tag{0.1}$$

Here W^h is the elastic energy density describing a composite material, $\nabla_h y^h = (\partial_1 y^h \mid \frac{1}{h}\partial_2 y^h \mid \frac{1}{h}\partial_3 y^h)$ denotes the scaled gradient of the deformation, and f^h describes an external load. Different scalings with respect to the thickness h in the applied load and elastic energy lead at the limit to different rod models [3, 5]. We consider the *von Kármán scaling*, i.e. a minimizing sequence (y^h) satisfies

$$\limsup_{h\downarrow 0} \frac{1}{h^4} \int_\Omega W^h(x, \nabla_h y^h)\mathrm{d}x < \infty\,, \tag{0.2}$$

while the forcing term scales as $f^h = h^3 f$ with $f \in L^2((0, L), \mathbb{R}^3)$. Under assumption (0.2) one can prove, using the rigidity estimate [2], that minimizers y^h of $\mathcal{E}^h$ are close to a rigid body motion and its rigid transformations $\hat{y}^h$ converge to the identity on $(0, L)$ in the L^2-norm [4]. Furthermore, sequences of scaled displacements (u^h), (v_2^h), (v_3^h) and twist functions (w^h), defined by:

$$u^h(x_1) = \int_\omega \frac{\hat{y}_1^h - x_1}{h^2}\mathrm{d}x'\,, \quad v_i^h(x_1) = \int_\omega \frac{\hat{y}_i^h}{h}\mathrm{d}x'\,,\ i = 2, 3\,, \quad w^h(x_1) = \int_\omega \frac{x_2\hat{y}_3^h - x_3\hat{y}_2^h}{h^2}\mathrm{d}x'$$

converge weakly (on a subsequence) to $(u, v_2, v_3, w) \in H^1(0, L) \times H^2(0, L) \times H^2(0, L) \times H^1(0, L)$. Our work asserts that if $\hat{y}^h$ are also stationary points of $\mathcal{E}^h$ (in addition to being minimizers), i.e. $\hat{y}^h$ solves the Euler–Lagrange equation

$$\int_\Omega \Big(DW^h(x, \nabla_h y^h) : \nabla_h \phi - h^3(f_2\phi_2 + f_3\phi_3) \Big)\,\mathrm{d}x = 0\,, \tag{0.3}$$

for all test functions $\phi \in H^1_\omega(\Omega, \mathbb{R}^3) = \{\phi \in H^1(\Omega)\ :\ \phi|_{\{0\}\times\omega} = 0\}$, then (u, v_2, v_3, w) is a stationary point of the functional $\mathcal{E}^0$, which is the Γ-limit of the sequence of functionals $(\mathcal{E}^h)$ [1].

Keywords: elasticity, homogenization, dimension reduction, convergence of equilibria.
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Asymptotic analysis of viscoelastic shells

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In this work we use the asymptotic expansion method in order to obtain two-dimensional limit models for viscoelastic shells. To do that, we first consider a family of linear viscoelastic shells with thickness 2ε (where ε is a small parameter that tends to zero) all having the same middle surface S and subjected to a boundary condition of place along a portion of their lateral face. Particularly, we present results that ensure the existence and uniqueness of solution of the corresponding variational formulation in curvilinear coordinates. We then suppose the existence of an asymptotic expansion of the solution (displacements). Upon substitution into the variational equations, we proceed to identify the terms of the proposed asymptotic expansion. In particular, we find that the zeroth-order term is the solution of a two-dimensional limit problem. Specifically, we distinguish two different limit formulations, depending on the order of the applied forces. We reproduce the terminology of the elastic shells to denote these two formulations as viscoelastic membrane shells and viscoelastic flexural shells, respectively. In both cases we find a model which includes a long term memory, thus taking into account the deformations at previous times. Finally, we comment the existence and uniqueness of solutions of the limit problems in the original domain and advance convergence results which fully justify the limit models found here.

Keywords: Asymptotic Analysis, Viscoelasticity, Shells, Membrane, Flexural, Time dependent.
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Homogenization of a hyperbolic-parabolic problem in a perforated domain

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We study the homogenization of the hyperbolic-parabolic system

$$\begin{aligned}
\partial_{tt}^2 u_\varepsilon(x,t) + \partial_t u_\varepsilon(x,t) - \nabla \cdot \left(a\Big(\frac{x}{\varepsilon}, \frac{t}{\varepsilon}\Big) \nabla u_\varepsilon(x,t) \right) &= f_\varepsilon(x,t) \text{ in } \Omega_\varepsilon \times (0,T), \\
a\Big(\frac{x}{\varepsilon}, \frac{t}{\varepsilon}\Big) \nabla u_\varepsilon(x,t) \cdot n &= 0 \text{ on } \partial\Omega_\varepsilon - \partial\Omega, \\
u_\varepsilon(x,t) &= 0 \text{ on } \partial\Omega \times (0,T), \\
u_\varepsilon(x,0) &= g_\varepsilon(x) \text{ in } \Omega_\varepsilon \\
\partial_t u_\varepsilon(x,0) &= h_\varepsilon(x) \text{ in } \Omega_\varepsilon
\end{aligned}$$

by means of adaptions of the evolution setting of multiscale convergence and very weak multiscale convergence [1] to periodically perforated domains Ω_ε [2]. Such domains mean that periodically arranged identical holes appearing with a period of characteristic size ε have been removed from an open bounded set $\Omega \subset \mathbb{R}^N$ except in the layer closest to the boundary $\partial\Omega$ .The set $\partial\Omega_\varepsilon - \partial\Omega$ means the boundary of these holes and the coefficient $a(y,s)$ is periodic with respect to $(0,1)^N \times (0,1)$. Moreover, let Y^* be the upscaling of one period of the perforated domain Ω_ε to the size of a unit cube and $\theta = \mu(Y^*)$. Under certain assumptions on the convergence of $\{f_\varepsilon\}$, $\{g_\varepsilon\}$ and $\{h_\varepsilon\}$, $\{u_\varepsilon\}$ approaches the solution u to the homogenized system

$$\begin{aligned}
\theta\partial_{tt}^2 u(x,t) + \theta\partial_t u(x,t) - \nabla \cdot (b\nabla u(x,t)) &= f(x,t) \text{ in } \Omega \times (0,T), \\
u(x,t) &= 0 \text{ on } \partial\Omega \times (0,T), \\
u(x,0) &= g(x) \text{ in } \Omega, \\
\partial_t u(x,0) &= \theta^{-1} h(x) \text{ in } \Omega
\end{aligned}$$

for $\varepsilon \to 0$. The homogenized coefficient b is identified by the local problem

$$\begin{aligned}
\partial_{ss}^2 u_1(x,t,y,s) - \nabla_y \cdot \big(a(y,s) \left(\nabla u(x,t) + \nabla_y u_1(x,t,y,s) \right) \big) &= 0 \text{ in } \Omega \times (0,T) \times Y^* \times (0,1), \\
a(y,s) \left(\nabla u(x,t) + \nabla_y u_1(x,t,y,s) \right) \cdot n &= 0 \text{ on } \Omega \times (0,T) \times (\partial Y^* - \partial Y)
\end{aligned}$$

through

$$b\nabla u(x,t) = \int_0^1 \int_{Y^*} a(y,s) \left(\nabla u(x,t) + \nabla_y u_1(x,t,y,s) \right) dyds.$$

Keywords: Homogenization, parabolic, hyperbolic, perforated domains.

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Homogenization of a hyperbolic-parabolic problem with three spatial and three temporal scales

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We study the homogenization of the hyperbolic-parabolic system

$$\begin{aligned}\partial_{tt}^2 u_\varepsilon(x,t) + \partial_t u_\varepsilon(x,t) - \nabla\cdot\left(a\Big(\frac{x}{\varepsilon},\frac{x}{\varepsilon^2},\frac{t}{\varepsilon},\frac{t}{\varepsilon^3}\Big)\nabla u_\varepsilon(x,t)\right) &= f(x,t) \text{ in } \Omega\times(0,T),\\ u_\varepsilon(x,t) &= 0 \text{ on } \partial\Omega\times(0,T),\\ u_\varepsilon(x,0) &= g(x) \text{ in } \Omega,\\ \partial_t u_\varepsilon(x,0) &= h(x) \text{ in } \Omega\end{aligned}$$

by means of general methods of multiscale convergence and very weak multiscale convergence adapted to an evolution setting [1]. When ε passes to zero $\{u_\varepsilon\}$ converges in a certain sense to the solution u to the homogenized system

$$\begin{aligned}\partial_{tt}^2 u(x,t) + \partial_t u(x,t) - \nabla\cdot(b\nabla u(x,t)) &= f(x,t) \text{ in } \Omega\times(0,T),\\ u(x,t) &= 0 \text{ on } \partial\Omega\times(0,T),\\ u(x,0) &= g(x) \text{ in } \Omega,\\ \partial_t u(x,0) &= h(x) \text{ in } \Omega.\end{aligned}$$

The homogenized coefficient b is identified by the local problems

$$\begin{aligned}-\nabla_{y_2}\cdot\left(\left(\int_0^1 a(y_1,y_2,s_1,s_2)ds_2\right)(\nabla u+\nabla_{y_1}u_1+\nabla_{y_2}u_2)\right) &= 0,\\ \partial_{s_1s_1}^2 u_1 - \nabla_{y_1}\cdot\int_{Y_2}\left(\int_0^1 a(y_1,y_2,s_1,s_2)ds_2\right)(\nabla u+\nabla_{y_1}u_1+\nabla_{y_2}u_2)\,dy_2 &= 0,\end{aligned}$$

in $\Omega\times(0,T)\times Y_1\times Y_2\times(0,1)$ and $\Omega\times(0,T)\times Y_1\times(0,1)$, respectively, through

$$b\nabla u(x,t) = \int_0^1\int_0^1\int_{Y_1}\int_{Y_2} a(y_1,y_2,s_1,s_2)\,(\nabla u+\nabla_{y_1}u_1+\nabla_{y_2}u_2)\,dy_2dy_1ds_2ds_1,$$

where $u=u(x,t)$, $u_1=u_1(x,t,y_1,s_1)$ and $u_2=u_2(x,t,y_1,y_2,s_1)$.

Keywords: Homogenization, multiscale convergence, hyperbolic, parabolic.

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Mathematical modelling of calcium signalling taking into account mechanical effects

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Most of the calcium in the body is stored in the bones. The rest is stored elsewhere, and calcium signalling is one of the most important mechanisms of information propagation in the body. Yet, many questions are still open and mathematical modelling can help answer them; several models of calcium signalling have been proposed, see for example [1]. In this work, we initially consider the model by Atri et al. [2]. When we omit calcium diffusion, this model is a system of two nonlinear ODEs for the calcium concentration, and the fraction of IP_3 receptors that have not been inactivated by the calcium.

We analyse in detail the bifurcations that arise in this model as the IP_3 concentration, the *bifurcation parameter*, is increased. The system exhibits relaxation oscillations for a finite range of the bifurcation parameter. Calcium oscillations are thought to control a wide variety of cellular processes, and are often organised into intracellular and intercellular calcium waves. To further study the relaxation oscillations that arise, we exploit a separation of timescales and we develop an appropriate asymptotic analysis [3].

Furthermore, motivated by experimental evidence that cells release calcium when mechanically stimulated and that, in turn, calcium release affects the mechanical behaviour of tissue, we propose an extension of the 2D system to a 3D ODE system. The third variable models the dilatation of tissue, and we also introduce a mechanical stimulus that induces calcium release. We now have two bifurcation parameters; the IP_3 concentration, as previously, and the strength of the mechanical stimulus, and we study the system and the bifurcations that arise. We investigate in detail the interplay of the mechanical and the chemical effects; we find that as the strength of the mechanical stimulus increases, the IP_3 parameter range for which oscillations emerge decreases until oscillations eventually vanish at a critical value of the mechanical stimulus. Furthermore, we again exploit a separation of timescales and we study the nonlinear 3D system asymptotically.

Keywords: modelling, calcium signalling, mathematical biology, excitable system, asymptotic methods

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CT07: Numerical simulation on solid mechanics

Evaluation of steel buildings by means of non-destructive testing methods

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Non-destructive testing methods became popular within the last few years. For steel beams shored in buildings there are currently only destructive ways for testing the yield limit as well as for determination of the current stress level. Rise of ultrasonic and micro-magnetic tools for (non-destructive) measurements allows the characterization of the inbuild material especially old steel bridges as economical and economical menance of the infrastructure.

Inbuilded steel beams are inhomogeneous, under stress and have typically unhandable surfaces leading to measurements afficted with errors. Our solution was the use of adapted statistical tests, a median-based outlier-test, to get a valid dataset. A further step, using non-causal time series, has been made to reduce in-data dependencies, probably caused by the measuring devices or the production process. The estimation of the stress curve was done with a kubic spline based regression approach which has shown an unexpected behaviour of the residuals. Further test has shown that there are again dependencies between different points of measurements. A non-causal time series approach solved that problem and further led to monte-carlo based confidence bands which has to be adapted to the valid standard.

Combining ultrasonic and micromagnetic data, gaining new dependency structures, an increase of the qualitiy of the estimation is observed. This is used to estimate all internal forces of the steel beam in face of dependend data. Bad numerical condition of the numerical procedures caused by dependencies inhibited that in the simple case without combination which is technically challenging in practice.

Proving the load carrying capacity of buldings according to valid standards will then be possible, more precise and much cheaper than the current state-of-the-art.

Keywords: Non-destructive Testing, Material Characterization, Time Series, Regime Switch, Heteroskedasticity, Monte Carlo
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Application of a Wiener Chaos Expansion approach for a slender inextensible elastic fiber driven by stochastic forces

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We examine the applicability of a Wiener Chaos Expansion (WCE) method in the case of an inextensible, elastic, slender, short fiber suspended in a turbulent air flow. The fiber is modelled as a 1d-parametrized, time-dependent curve, whose dynamics are given by a stochastic partial differential equation subject to an algebraic constraint. The stochastic forces raise from the turbulence of the surrounding air flow and are modeled by a space-time white noise, whose amplitude depends on the turbulent kinetic energy and dissipation rate of the flow [1]. Using a Finite Volume approach, one arrives at a constrained stochastic differential equation (SDE) system driven by a planar Wiener process [2]. The solution of SDEs by a WCE-based method has the advantage of an effective splitting between deterministic and stochastic effects, allowing an efficient calculation of the mean behavior of the system under consideration [3]. It is therefore of great interest, if such approaches are also applicable to SDEs with an algebraic constraint, which arise e.g. in the industrial fabrication of nonwovens [4].

Keywords: fiber suspension, Wiener-Chaos-Expansion, stochastic partial differential algebraic equations

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Stochastic fiber dynamics in a spatially semi-discrete setting – the case of a non-linear air drag model

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In this talk a simplified model for fiber dynamics in turbulent airflow will be presented and analyzed. Modeling these dynamics with a focus on the production of nonwoven-textiles is a scientific issue for over one decade. In applications it is crucial to understand these dynamics since certain properties of the outcome product highly depend on it.

There exist no results concerning the analysis of the full space-time model up to this point. Recently, we introduced a simplified spatially semi-discrete model for which we analyzed the global solvability as well as numerical time discretization schemes, see [1]. The analysis was based on a linear underlying air drag model. In this talk these results will be generalized to a more realistic non-linear air drag model, which is similar to the one used at the Fraunhofer ITWM. We thereby bring the simplified model closer to industrial applications.

Keywords: Inextensible fiber dynamics, stochastic differential equations on manifolds

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Efficient and robust co-simulation of geometrically exact Cosserat rod model and multibody system

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In modern system simulation, the increasing complexity and level of detail in the formulation of single subsystems is a challenging task for the numerical integration. To achieve efficient simulation, often co-simulation is used, i.e. the subsystems are solved with especially suited numerical methods and data is only exchanged at discrete points in time. Moreover, this allows to perform the numerical integration of subsystems in parallel and, thus, additionally saves computation time.
Unfortunately, co-simulation may result in unstable numerical simulation. This is the case, if algebraic loops arise due to the data exchange [1, 2]. One way out are, e.g., implicit co-simulation schemes, which, however, are computationally expensive.
Our main focus is the fast simulation of slender components, like cables and hoses, in vehicle dynamics. Thus, we kinematically couple a very efficient and geometrically exact Cosserat rod model [3] with classical rigid multibody systems. In order to do so, we describe the kinematic coupling by an algebraic constraint, which enables a simple formulation of different coupling joints. From this constraint coupling, an efficient force-displacement co-simulation scheme is developed [4], which performs explicitly and in parallel. We want to remark, that our coupling strategy could also be applied to arbitrary kinematically coupled mechanical subsystems, and especially to kinematic couplings in flexible multibody dynamics.
It turns out, that the mass ratio of the coupled masses of the subsystems is decisive for stable co-simulation. Modifying the masses of the multibody system to improve the mass ratio would also change the system dynamics. In contrast, the coupled mass of the flexible structure can be changed by modifying the spatial discretization of the cable model, without varying the physical properties. In particular, a refined discretization leads to stable co-simulation. For equidistant spatial discretization, this might lead to a drastically increasing number of degrees of freedom. Thus, only a local refinement close to the coupling interface would be preferable.
How this behaves for the complex cable model is part of our current research.

Keywords: multibody dynamics, flexible structures, constraint coupling, co-simulation.

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Application of critical J-integral as fracture criterion to model resistance spot weld failure in martensitic boron steels.

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The load bearing capacity of joints during crash tests is of great importance for the design of new vehicles in the automotive industry. Among all joining technologies, resistance spot welding is the most popular joining technique. With the introduction of Advance High Strength Steels (AHSS) the bearing capacity of the vehicle parts increased and the importance of the fracture behaviour of joints became even higher.

The joints bearing capacity in common ductile steels is typically restricted by the base material mechanical properties around the weld nugget and is usually linearly dependent on the steel fracture strength. However, in AHSS the material properties are modified around the joint due to the welding process and new critical failure zones are introduced. During the last years detailed finite element models of spot welds along with very detailed characterization of fracture strains of different spot weld zones were used to predict loading maximum forces in AHSS.

However, in the case of martensitic boron steels, due to the mechanical properties distribution, the critical failure zone in most of loading cases is a notch generated during the welding process. Around this notch, high stress and strains gradients are produced during loading, and the accuracy of FEM solution is lower and very mesh dependent. Detailed characterization of fracture strains cannot be used as fracture criterion any more.

In this work the strain energy release rate is calculated using J-integral to evaluate the severity of the stress concentration and compared with the material fracture toughness, to get the applied forces when crack nucleates and the joint fails. J-integral is evaluated from the results gathered from FEM simulations using the equivalent domain integral method implemented for 3D 8-node elements with 1 x 1 x 1 Gauss integration points.

The model was calibrated and calculated using welded specimens, of different thickness combinations, spot weld diameters and loading angles giving very promising results.

Keywords: finite elements method fracture mechanics J-integral resistance spot welding martensitic boron steel

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CT08: Biomedicine applications

A variational model and algorithm for adaptive reconstruction of x-ray radiographs

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X-ray radiography is an excellent tool for peering into the interior of an object. X-ray radiograph is a digitized image. Image reconstruction means to recover the object physical features from line-integral measurements through the object. For fixed experimental system, the accuracy of image reconstruction depends much on the mathematical model and algorithm. This work focus on the Abel transform inversion based image reconstruction from noisy and blurred projection data. This is an ill-posed problem. To overcome the ill-posedness, both Laplacian and Total Variation regularizers are jointly considered. A variational model is proposed to adaptively recover the image edges and smooth regions. Numerical results illustrate the efficiency and accuracy of our proposed model. It has advantages on staircasing reduction, contrast preservation and SNR value improvement.

Keywords: Image Reconstruction, x-ray Tomography, Abel Transform, Total Variation, Inverse Problem.
Acknowledgments. Partially supported by NSFC project No. 11571003.

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Solutions to Fokker/Planck equations in 1D slab geometry

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Recently, Ó. López Pouso and N. Jumaniyazov presented in [1] a new numerical scheme of order 2 for solving the two/way degenerate diffusion problem

$$\mu\frac{\partial\psi}{\partial z}+\alpha\psi-\sigma\frac{\partial}{\partial\mu}\left[\left(1-\mu^2\right)\frac{\partial\psi}{\partial\mu}\right]=W \text{ for } (\mu,z)\in Q=[-1,1]\times[Z_{\text{ini}},Z_{\text{fin}}], \tag{0.1}$$

$$\psi(\mu,Z_{\text{ini}})=f(\mu) \text{ for } \mu\in(0,1], \tag{0.2}$$

$$\psi(\mu,Z_{\text{fin}})=g(\mu) \text{ for } \mu\in[-1,0). \tag{0.3}$$

In this problem, function $\psi:(\mu,z)\in Q\to\psi(\mu,z)\in\mathbb{R}$ is the unknown, $Z_{\text{ini}}<Z_{\text{fin}}$ are real numbers, and functions $\alpha,\ \sigma,\ W,\ f$ and g are known. Data functions $\alpha,\ \sigma$ and W are allowed depending on (μ,z). In the context of nuclear engineering, the PDE (0.1) is the well/known monoenergetic (i.e., energy independent) steady Fokker/Planck equation in the 1D slab with planar/geometry symmetry (i.e., azimuthal angle independent), while W is a source/sink term and $\frac{\partial}{\partial\mu}\left[\left(1-\mu^2\right)\frac{\partial\cdot}{\partial\mu}\right]$ is the so/called continuous/scattering operator. Equations (0.2) and (0.3) are the incoming flux boundary conditions. The importance of this problem lies in that its solution is an approximation of the solution to the Boltzmann transport equation, whose computation is much more expensive, for particles that suffer highly forward/peaked scattering and small energy losses. Typical examples are charged particles like electrons or heavy ions. In this context, ψ represents the angular flux density of particles.

On the basis of numerical experiments, the behaviour of the López Pouso/Jumaniyazov scheme, when applied to the time dependent problem, the energy dependent problem, and the azimuthal angle dependent problem, will be discussed.

Keywords: electron transport, Fokker/Planck equation, 1D slab, time dependent problem, energy dependent problem, azimuthal angle dependent problem.

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A competitive random sequential adsorption model for immunoassay activity

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Immunodiagnostic devices (or immunoassays) rely on the binding of antigens by antibodies and are used to detect biomarkers for a variety of diseases with high specificity, in a range of media including blood or urine. Many immunoassay technologies involve immobilization of the antibody to solid surfaces (this configuration also occurs on a large scale in physiological reactions *in vivo*). One of the primary design considerations in such cases is optimizing the concentration of capture antibody in order to achieve maximal antigen binding and, subsequently, improved sensitivity and limit of detection.

The theory known as *random sequential adsorbtion* (RSA) has been successfully used over the past few decades to describe monolayer particle deposition, with wide applications in many physical and biological settings ([1] [2], [3]). A generalization known as competitive RSA (see, for example, [4]) deals with mixtures of particles having different sizes and adsorption probabilities. Within this framework, we propose a few mathematical models of varying difficulty (taking into account different antibody geometries or possibility of overlap) which quantify the assay activity by calculating the concentration of correctly oriented particles (active site exposed for subsequent reactions) and its dependence on system parameters. This is achieved by solving evolution equations of integro-differential type for various gap length density functions. The signal is then determined from the reaction product, which provides a qualitative comparison to experimental calibration curves.

It has been suggested by experimental studies (for example, [5] [6]) that high immobilized antibody concentrations will decrease the assay performance, due to molecule denaturation and obstruction of active binding sites. However, crowding of particles can also have the opposite effect by favouring upright orientations. We therefore attempt to predict which of these competing effects prevails under different experimental conditions and find the coverage which yields the maximum expected concentration of active particles (and hence the highest signal).

Keywords: Random sequential adsorption, immunodiagnostic devices, immobilized particles, integro-differential equations.
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CT09: Dynamical systems

Mathematical modeling and dynamic behavior of a new self-excited microfluidic oscillator

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This work is concerned with the modeling and dynamical study of a self-excited chemo-fluidic oscillator recently developed in [1]. This device has the potential ability of coupling chemical, biochemical or biological systems with fluidic systems, which expands the possibilities towards smart processing of chemical information in a microfluidic environment. The main component in the considered chemo-fluidic oscillator is a microfluidic valve, which consists of a particle of a stimuli-responsive (smart) hydrogel placed in a valve seat formed in a microfluidic channel. Due to its volume phase transition behavior, a smart hydrogel has the capacity to change its volume under small variations of special thermodynamic parameters, in a reversible and reproducible manner. In our investigation, the volume of the hydrogel is controlled via the concentration of alcohol at the hydrogel junction, which, as a consequence, opens and closes the microfluidic valve [2].

The chemo-fluidic oscillator considered here is based on a negative feedback loop containing a delay line, where the negative feedback is provided by the hydrogel valve. The hydrogel is designed in such a way that an increment of the alcohol concentration reduces the size of the hydrogel and vice versa. Therefore, at low alcohol concentrations the hydrogel valve is closed, while high alcohol concentrations open the valve. One of the main challenges in this investigation is to estimate the parameters of the system that would allow stable oscillations to occur, for a wide range of operational conditions, with particular care regarding available laboratory equipment, fabrication constraints and safe operation ranges suggested by components manufacturers.

In this presentation we introduce a piecewise-smooth dynamical system describing the behavior of this chemo-fluidic oscillator. The periodic response of the model is studied by means of path-following techniques for non-smooth systems [3, Chapter 9]. Our investigation reveals that the origin of the oscillatory behavior is connected to the presence of a Hopf bifurcation in the system. Furthermore, the effect of several system parameters on the frequency of oscillation is studied in detail.

Keywords: Chemo-fluidic oscillator; Non-smooth dynamical system; Numerical continuation.

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Structure preserving numerical schemes for population dynamics models

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In population biology the multi-particle systems for different species can be described in the continuum limit by cross-diffusion systems derived from lattice models. In this way one get strongly coupled system of nonlinear parabolic PDEs whose diffusion matrix is often neither symmetric nor positive definite. These challenging mathematical difficulties can be overcomed if the analysed cross-diffusion model possess a gradient-flow structure.

In this talk we present numerical discretization which preserve the entropy structure of the Shigesada-Kawasaki-Teramoto (SKT) cross diffusion model. The main features of the proposed discretization are the preservation of the non-negativity and the entropy-dissipation structure. The main idea is to combine Dahlquist's G-stability theory with entropy dissipation methods. Entropy dissipation techniques were intensively used in the mathematical analysis of PDEs for derivation of apriori estimates which represent a crucial tool in proving the existence of solutions and studying their long-time behavior.

We prove the existence of semi-discrete weak solutions of proposed one-leg multi-step time discretization. The optimal second-order convergence rate is proved under a certain monotonicity assumption on the operator. We note that our results can also be applied to some higher-order nonlinear evolution equations arising in semiconductor modelling.

Keywords: strongly coupled parabolic systems, entropy dissipation, gradient flow, linear multistep methods
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CT10: ODEs

Symmetric solutions in delay-coupled laser networks with all-to-all coupling

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A network of semiconductor lasers is considered where each laser receives a feedback light from all other lasers in the network. The model is described using the Lang-Kobayashi rate equations [1, 4] where the finite propagation time of the light from one laser to another is reflected by a constant delay time parameter in the laser optical fields. Due to the network structure, the resulting system of delay differential equations has symmetry group $\mathbf{S}_n \times \mathbf{S}^1$. Our result classifies all types of symmetric solutions to the system. This is done by characterizing all isotropy subgroups [5] of the symmetry group $\mathbf{S}_n \times \mathbf{S}^1$. Branches of symmetric solutions, i.e. solutions fixed by isotropy subgroups, are then obtained using DDE-Biftool [3]. This work complements the author's previous work [2] which identifies symmetry-breaking bifurcations in the same laser network with all-to-all coupling.

Keywords: Lang-Kobayashi equations, symmetry, all-to-all coupling, semiconductor laser, networks
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Nutrient cycling in an agricultural setting

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Phosphate (P) and sulphate (S) are essential nutrients for plant growth [1]. However, the only natural source of P is the slow chemical weathering of phosphate-bearing rocks. This supply is unable to meet the demands of modern agriculture, potentially leading to a phosphate crisis [2]. Though plants can absorb sulphur dioxide directly through their leaves, cropped soils are nonetheless likely to experience sulphur deficiency without additional S input from the atmosphere or fertilizers [3]. In order to manage soil nutrient resources in the long term, a better understanding of soil-plant nutrient cycles is required.

The recycling of nutrients through the deposition and subsequent decomposition of leaf litter plays an important role in ensuring sustained P and S supply. The activity of soil microbes is also required in order to convert P and S into forms that are directly available for plant uptake. In particular, bacteria and fungi metabolise organic compounds containing P and S and in the process, release inorganic forms of the nutrients that are available for plant uptake [4]. The decomposition of leaf litter also depends on microbial metabolism. Moreover, mycorrhizal fungi facilitate the transport of nutrients from the soil to the plant root in exchange for carbon.

We propose differential-equation based models of P and S cycling at the scale of a single plant. These models explicitly include the returning of nutrients from plants to the ground surface as well as the aforementioned microbe-mediated conversions in the soil. Using this model, we aim to develop a qualitative and quantitative understanding of biologically mediated cycling effects as well as the abundance and bio-availability of P and S throughout the depth of a soil profile. This includes examining the time scales of microbial growth and nutrient cycling as well as looking at the symbiotic phosphorus-carbon exchange between plants and mycorrhizae.

Our P and S models are being developed in tandem with a series of experiments carried out at the Department of Life Sciences at the University of Limerick and by the agriculture and food development authority, Teagasc. Lab experiments involve planting soil columns with English ryegrass and applying phosphate and sulphate fertilizers. The abundance of these nutrients in soil solution, root biomass and microbial biomass will be measured and this data will be used to guide model design and estimate parameter values. Some preliminary modelling and experimental results will be presented in this talk.

Keywords: nutrients, cycling, phosphate, sulphate, agriculture, microbes
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CT11: Population dynamics

Opinion dynamics in the presence of external manipulation

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Public opinion underpins many important decisions that occur in society, from who best to lead a country, to how to tackle climate change. Understanding the dynamics of opinion formation, and how best to manipulate these opinions, has therefore been of central interest to a wide range of groups, from social science researchers, to company marketing departments.

There are many elements which may influence the development of an opinion, such as personality, culture and peer interaction, however attempts have been made to capture the key features of the resulting dynamics with relatively simple models. Perhaps the simplest is the voter model [1], which assumes people hold one of two opinions and that they can change their opinion on interaction with their neighbours. Attempts to move beyond this binary model have included introducing a wider range of discrete choices [2], a continuous scale for opinions [3], and the possibility of disagreement between neighbours [4]. Most models however are stochastic in nature, relying on shifts in opinion with some probability.

In this work I introduce a model of continuous opinion which incorporates nonlinear interactions between players to model the opinion dynamics. Within this dynamical systems framework I examine a number of problems in social dynamics. In the presence of both agreement and disagreement I show that extreme opinions may spontaneously appear in the population. I explore the effect of interactions with a global player ("the government"), which has a fixed external opinion relative to the population, and identify the optimal strategy for this player to generate support, finding that success in this manipulation may occur at the cost of an increase in extremism. I also examine the problem of opinion dynamics when players have some choice in which opinions to listen to, for instance relevant to opinions on vaccination/anti-vaccination, and explore possible approaches to modelling this more complex situation, again in the presence of external players which are seeking to manipulate the overall public opinion.

Keywords: mathematical modelling, social dynamics, opinion spread, extremism

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Mathematical modeling of malware propagation in critical infrastructures

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As is well known critical infrastructures are essential for the maintenance of the basic social requirements and their abnormal function or destruction would have a significant impact both on governments and private companies as well as on the health, safety, security and economic well-being of citizens. The information and telecommunication technologies play a crucial role in the control and operation of several processes in critical infrastructures, and its use has resulted in innumerable benefits. However, this scenario is not without threats, and the most important and dangerous is the presence of malware in the network of a critical infrastructure [1].

Malware is software created to carry out unauthorized (and, usually, malicious) activities in the devices of computer networks and, consequently, it is very important not only to detect the existence of malware in the network but also to simulate in a proper way its propagation over the whole network.

Although several mathematical models have appeared in the scientific literature in order to simulate malware propagation in different environments: computer networks, mobile networks, wireless sensor networks, etc. ([2, 3]), unfortunately (and as far as we know) there is not any model devoted to the study of malware spreading in critical infrastructures. The critical infrastructure networks have some particular characteristics that make them different from the rest, and in this sense it is mandatory to design specific mathematical models that take them into account.

The main goal of this work is to propose a novel mathematical model to simulate malware spreading in a critical infrastructure network. As networks have similarities with individual-based spatial models, our proposal is based in this paradigm: each device of the network stands for a node of the graph associated to the network topology, and each edge stands for a connection between the nodes/devices considered. Moreover, the network structure defines some coefficients of the model such as the force of infection and the recovery rate. Also population dynamic (the replacement of disrupt devices) is considered.

The basic reproductive number is explicitly derived and analyzed. Moreover, both the malware-free equilibrium point and the malware-endemic equilibrium point are computed and consequently the stability analysis of the model is presented. In this sense, a theoretical study of the best control strategies is performed, and several simulations are computed to illustrate the theoretical results.

Keywords: Malware propagation, mathematical modeling, critical infrastructures, epidemics on networks.
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Mathematical models with generic birth and death rates in population dynamics with applications in biotechnology and ecology

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Mathematical modelling is an important tool in population dynamics that allows describing various biotechnological and ecological processes.

The classical models (e.g., the Monod-type models, modelling microbial growth or the Rosenzweig-MacArthur predator-prey model, among others) assume a per capita growth rate that is linear w.r.t. the food intake and a constant per capita death rate.

In the present work, we consider generic birth and death rates based on several observations proposed by A.J. Terry in [1].

For sufficiently small values of the consumption, the reproduction will be zero rather than linearly increasing. Also, there will always be a limit to the rate at which an individual can reproduce.

On the other hand, every organism needs some minimal energy intake, in order to survive. Therefore, under this threshold the death rate should be higher.

Using the idea of non-linear birth and death rates, we propose models that are generalizations of classical models in population dynamics. We study the asymptotic properties of the solutions of the considered models. We show that in some cases those models have much richer dynamics and, thus, allow us to model more complex behaviour of the biological system.

Also, we investigate their ability to model real processes by comparing the results of the parametric identification process to experimental data for different microbial cultures.

Keywords: Population dynamics, microbial growth, predator-prey, biotechnology, stability analysis.

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CT12: Chemical kinetic models

Parameters inference in chemical reactions networks. Model selection and missing data.

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Model inference is a challenging problem in the analysis of chemical reactions networks. In order to empirically test which, out of a catalogue of proposed kinetic models, is governing a network of chemical reactions, the user can compare the empirical data obtained in one experiment against the theoretical values suggested by the models under consideration. It is thus fundamental to make an adequate choice of the control variables (e.g. initial concentrations of the different species in the tank) in order to have maximal separation between sets of concentrations provided by the theoretical models, making then easier to identify which of the theoretical models yields data closest to those obtained empirically under identical conditions.

In this work we illustrate how Global Optimization techniques can be successfully used to address the problem of model separation, as a basis for model selection. Furthermore, these approaches can be used to deal with the problem of parameters inference when there exist missing values in the data sets. Some examples illustrate the usefulness of our methodology.

Keywords: model selection, missing data, chemical reactions networks, kinetic models, global optimization, Variable Neighborhood Search.

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A mathematical description of steady-state branched-chain thermal reaction with general temperature dependent rate law

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A numerical investigation is performed for the thermal parameter estimation in the mathematical model of a process based on initiation, chain branching and chain breaking kinetics arising from the hydrogen-oxygen mixture as well as acetylene-oxygen systems in a reactive slab. Assuming generalized Arrhenius kinetics, steady state theory and energy conservation in the adiabatic system resulted in nonlinear elliptic equation. The effect of sundry parameters such as initiation rate compared with the diffusion coefficient, order of the branching reaction and exponent of the pre-exponential factor on the critical values of self-ignition and extinction as well as transitional values of the associated physical parameters are compared with results in literature; graphical representations were explained and then discussed. The results help to enhance understanding of the interplay between thermal and branched-chain thermal explosions.

Keywords: Combustible mixture, Thermal explosions, Branched-chain thermal reaction, Shooting method.
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Predicting nitrate concentrations in soil borehole data

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The quality of groundwater is of immense interest worldwide with several legislation directives by various governments addressing the issues of pollution and protection. The maintenance of this resource was emphasized by a recent study which concluded that only approximately 6% of groundwater is renewable [Gleeson et al., 2015]. Groundwater contamination arises from spills and leaks which contaminate water locally, form a contaminant plume, and then migrate under the influence of groundwater flows. If these plumes reach streams, wells, or other sources of drinking water then this creates an overall potable water quality hazard.

Countering this contamination is the process of bioremediation whereby naturally occurring bacteria in soil consume pollutants, removing them from the groundwater plumes. It is therefore important to understand the impact and effectiveness of bioremediation on contaminant plumes in order to minimize the negative impact on water quality. One such way to do this is by digging boreholes in soil where contaminants are expected and then chemically analyzing the soil water found in these boreholes to look for concentrations of known pollutants (cf. [Smits et al., 2009]. [Davison, 1998]). However, collecting borehole data can be a very expensive process and a modelling approach may provide an inexpensive tool for understanding contaminant transport.

In this talk we will look at a set of borehole data from Mansfield, U.K. and analyze nitrate, a common contaminant found in plumes. We model nitrate via a series of reduction-oxidation (redox) reactions mediated by bacteria which consume or produce nitrate based on other soil nutrients. We will begin with a chemostat model where we ignore spatial influence and allow for a feed of nutrient into the system. Using this model we show how sustained oscillations between nitrate and bacterial populations can occur. We then consider a proper spatial model where nutrient diffusion is considered. In this model we show that there are two very clear regions, an oxygen rich region where aerobic bacteria thrive and produce a large spike of nitrate and an anoxic region where secondary bacteria maintain different nitrogen kinetics. When comparing the results to the borehole dataset we will show the presence of this double region behaviour.

Keywords: nutrient modelling, groundwater contamination, reaction diffusion kinetics.
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CT13: Finite volumes

Simulating heat and mass transfer with limited amount of sensor data

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We consider the problem of simulating heat and mass transfer inside a building. It is assumed that the building is equipped with a network of sparsely located sensors and a data management system that records sensor measurements of temperature, relative humidity, and air flow at fixed time intervals. The focus is on environments where natural convection must be accounted for in the heat and mass transfer process. To address the problem at hand, we propose a three-dimensional, time-dependent boundary value problem (BVP) for a mixture of two fluids, namely water vapor and dry air, as a model for simulating the distribution of temperature and concentration of water vapor in (humid) air inside a room (or more generally, a building). Sensor measurements serve as input to the model, in the form of time-dependent boundary data.

In addition to the model, emphasis is placed on a numerical solution approach that will facilitate integration of the proposed methodology as part of a data management system which, besides recording sensor measurements, could provide modeling and analytics capabilities to aid with aspects such as building energy management, design, and operational support. To this end we work with freely-available software for solving partial differential equations, specifically OpenFOAM [1] and NETGEN [2], and build upon the available capabilities as needed.

We present results from numerical simulations performed using a set of synthetic data representing a time series of temperature and relative humidity sensor measurements. The sensors are assumed to be few in number and sparsely located throughout the boundaries of a room. Significant improvements in the three-dimensional simulation results are obtained by considering first BVPs in two spatial dimensions to simulate the distribution of temperature and concentration of water vapor on the boundary of the three-dimensional domain. Coupled with the sensor data, the solution of these two-dimensional BVPs provide a mathematically and physically meaningful approach for prescribing boundary conditions for the three-dimensional model.

Future directions to pursue include incorporating additional terms in the two-dimensional BVPs in order to have a more detailed set of equations for the distribution of temperature and concentration of water vapor on the boundary. In addition, one should consider the use of real-time sensor measurements to calibrate the model and conduct further studies like, for example, the impact people may have on micro-climatic conditions and works of art housed in a museum [3]. From a computational point of view, it will be interesting to explore the use of multiple cores to perform the simulations using parallel computations. For instance, one could investigate how the proposed methodology scales up for whole building simulations by considering buildings with multiple (connected) rooms and performing the simulations in parallel by assigning one room per core.

Keywords: heat / mass transfer simulations, temperature / humidity sensor data

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Comparison of numerical schemes for the incompressible Navier-Stokes equations and convergence analysis

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The Crouzeix-Raviart scheme is one of the most used for the approximation of the incompressible Navier-Stokes equations. An advantage of this scheme is that the mass conservation equation can be seen as a finite volume equation, since the velocity is given at the center of the faces of the mesh. Although the implementation of this scheme for the Stokes problem is unique, this is not the case for the Navier-Stokes equations, due to the many possibilities for approximating the nonlinear convection term. Indeed, let us assume that the scheme is written under the following form:

$$\text{(0.1)} \qquad \left\{ \begin{array}{l} u \in X_{D,0}\,,\ p \in Y_{D,0}, \\ \displaystyle\int_\Omega \nabla_D u : \nabla_D v \ \mathrm{d}x + b_D(u,v) - \int_\Omega \Theta_D p \ \mathrm{div}_D v \mathrm{d}x = \int_\Omega f \cdot \Pi_D v \mathrm{d}x,\ \forall v \in X_{D,0} \\ \displaystyle\int_\Omega \Theta_D q \, \mathrm{div}_D u \mathrm{d}x = 0, \ \ \forall q \in Y_{D,0}, \end{array} \right.$$

where $d = 2$ or 3 is the dimension of space of the domain Ω, f is a source term of momentum, $X_{D,0}$ is the finite-dimensional vector space on $\mathbb{R}$ of the velocity degrees of freedom which vanish at the boundary of the domain, $Y_{D,0}$ the finite-dimensional vector space on $\mathbb{R}$ of the pressure degrees of freedom with null mean value, $\Pi_D u$ is the reconstruction of the approximate velocity field, $\nabla_D u$ is the discrete gradient field, $\mathrm{div}_D u$ is the discrete divergence field, $\Theta_D p$ is the discrete pressure field and $b_D(u,v)$ is an approximation of the nonlinear convection term $\sum_{i,j=1}^d \int_\Omega u_i(\partial_i u_j) v_j \ \mathrm{d}x$. A variety of expressions can be used for this term $b_D(u,v)$. In addition to the standard skew symmetric expression available in the finite element framework, different expressions may account for the discrete mass balance, in order to directly ensure the stability condition $b_D(u,u) \geq 0$.

We numerically compare different expressions on standard test cases (lid driven cavity, Poiseuille flow, analytical term with source term). We show that all of them can be interesting in various situations. We then turn to the convergence analysis of this family of schemes, remarking that this analysis can be extended to other families of discretisations (in particular the Taylor-Hood finite elements and the MAC scheme, which are important examples of schemes formulated with the velocity/pressure unknowns) thanks to the notion of gradient schemes (used in [1] in the case of the Stokes problem).

Keywords: Crouzeix-Raviart scheme, incompressible Navier-Stokes equations, gradient schemes.

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A conservative, hybrid hr-refinement strategy for a Finite Volume method on time-dependent domains

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Solutions of partial differential equations (PDEs) arising in science and industrial applications often undergo large variations occurring over small parts of a time-dependent domain. Resolving steep gradients and oscillations properly is a numerical challenge. The idea of the hybrid hr-refinement is to improve the approximation quality – while keeping the computational effort – by redistributing a variable amount of grid points in areas of the domain where they are needed and by controlling the amount of grid points through adding or removing them in a smooth manner at the boundary. This refinement is combined with a space-time Finite Volume method (1d in space) of first order on a staggered grid, the conservation properties are maintained. Numerical results are shown and applied to a fiber spinning process modelled by a partial differential-algebraic system of equations (PDAE).

Keywords: hr-refinement, moving mesh, conservative adaptivity, time-dependent domain, fiber spinning.
Acknowledgments. This work has been supported by German DFG, project 251706852, MA 4526/2-1, WE 2003/4-1.

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A convergent finite volume scheme of Darcy-Brinkman's velocities of two-phase flows in porous media

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Two phase flows in a porous medium model many interesting phenomena in geophysics. As exemples, we mention water flooding of oil reservoirs and carbon dioxide sequestration in subsurface formations.

Different empiric laws are used to describe the filtration of a fluid through porous media. Darcy law is the simplest and, by far, the most popular one, due to its simplicity. It states that the filtration velocity of the fluid is proportional to the pressure gradient. The Darcy law cannot sustain the no-slip condition on an impermeable wall or a transmission condition on the contact with free flow [1, 2].

That motivated H. Brinkmann in 1947 to modify the Darcy law in order to be able to impose the no-slip boundary condition on an obstacle submerged in porous medium. He assumed large permeability to compare his law with experimental data and assumed that the second viscosity μ equals the physical viscosity of the fluid in the case of monophasic flow. The Brinkman law could formally be obtained from the Stokes system describing the microscopic flow, by adding the resistance to the flow [3].

We are interested in the displacement of two incompressible phases in a Darcy-Brinkman flow in a porous media. The equations are obtained by the conservation of the mass and by considering the Brinkman regularization velocity of each phase. The mass conservation of two incompressible phases with Darcy-Brinkman velocity of each phase can be written in the following system (see [4, 5]).

$$
\begin{cases}
\phi\partial_t s - \phi\mu\Delta\partial_t s - \operatorname{div}\left(kf(s)\lambda(s)\nabla p\right) - \operatorname{div}\left(k\alpha(s)\nabla s\right) = 0 & \text{in } (0,T)\times\Omega \\
-\operatorname{div}\left(k\lambda(s)\nabla p\right) = 0 & \text{in } (0,T)\times\Omega \\
\displaystyle\int_\Omega p(t,x)\,\mathrm{d}x = 0 & \text{in } (0,T) \\
k\lambda(s)\nabla p(t,x)\cdot\eta = \pi(t,x) & \text{on } (0,T)\times\partial\Omega \\
\phi\mu\partial_\eta\partial_t s + f(s)\pi + k\alpha(s)\nabla s\cdot\eta = h(t,x) & \text{on } (0,T)\times\partial\Omega \\
s\left(0,\mathbf{x}\right) = s_0\left(\mathbf{x}\right) & \text{in } \Omega.
\end{cases}
\tag{0.1}
$$

This model is treated in its general form with the whole nonlinear terms. Our goal is the construction and convergence analysis of a finite volume scheme together with a phase-by-phase upstream according to the total velocity. Finally, numerical tests illustrate the behavior of the solutions of this proposed scheme.

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A dissipative discretization scheme for reaction-diffusion systems

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The structure size in lithography decreases with every new technology generation. Since extreme ultraviolet lithography is still not available, new combinations of the default exposure, post exposure, and development process steps are of interest. Another option is the creation of new lines by pattern self assembly. The modelling of such processes leads to reversible reactions of mass action type with diffusion, heterogeneous materials, and Neumann boundary conditions. The existence of heterogeneous materials can cause strong boundary layers in the solution.

For such typ of reactions a dissipative implicit Voronoi finite volume scheme is presented. It preserves the known analytic properties [1]: existence of a unique thermodynamic equilibrium solution, exponential decay of the free energy along trajectories towards thermodynamic equilibrium, existence of global bounded positive solutions and convergence to a weak solution [2, 3, 4]. The method is illustrated by a few examples with strongly varying timescales. The integral mass invariants of the kinetics are precisely preserved by the numerical algorithm. Timescales can be chosen such that the thermodynamic equilibrium is fifty orders of magnitude far away from the initial guess.

Keywords: lithography, post-exposure bake, reaction-diffusion systems, Voronoi finite volume scheme

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CT14: Heat transfer

Reduced Basis method applied to a convective instability problem

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The reduced basis approximation is a discretization method that can be implemented for solving of parameter-dependent problems $\mathcal{P}(\phi(\mu),\, \mu) = 0$ with parameter μ in cases of many queries. This method consists of approximating the solution $\phi(\mu)$ of $\mathcal{P}(\phi(\mu),\, \mu) = 0$ by a linear combination of *appropriate* preliminary computed solutions $\phi(\mu_i)$ with $i = 1, 2, ..., N$ such that μ_i are parameters chosen by an iterative procedure using the *kolmogorov n-width* measures [2, 4].

In [1], the reduced basis method is applied to a two dimensional incompressible Navier-Stokes equations with constant viscosity and the Boussinesq approximation coupled with a heat equation that depends on the Rayleigh number, $\mathcal{P}\,(\phi(R),\, R) = \vec{0}$.

Rayleigh-Bénard convection problem displays multiple steady solutions and bifurcations by varying the Rayleigh number, therefore the eigenvalue problem of the corresponding linear stability analysis has to be implemented. A linear stability analysis of these solutions is performed in [3] by Legendre spectral collocation method.

In this work the eigenvalue problem of the corresponding linear stability analysis is solved with the reduced basis method. It is considered the aspect ratio $\Gamma = 3.495$ and R varies in $[1,000;\, 3,000]$ where different stable and unstable bifurcartion branches appear [1, 3]. We apply the reduced basis method within this framework to compute whole bifurcation diagram with the stable and unstable solutions corresponding to many values of R in an interval of the considered bifurcation parameter. The reduced basis method permits to obtain the bifurcation diagrams with much lower computational cost.

The problem is numerically solved by the Galerkin variational formulation using the Legendre Gauss-Lobatto quadrature formulas together with the reduced basis $\{\phi(R_i), i = 1, 2, ..., N\}$ such that $\phi(R) \sim \sum_{i=1}^{N} \lambda_i \phi(R_i)$.

Keywords: Reduced Basis approximation, Bifurcation, Rayleigh-Bénard, Kolmogorov width, Flow problem, Model Reduction.
Acknowledgments. This work was partially supported by the Research Grants MINECO (Spanish Government) MTM2012-37642, PEII-2014-006-A (Castilla-La Mancha regional Government) and GI20152914 (Universidad de Castilla-La Mancha) which include RDEF funds.

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Effects of ambient rotation and temperature gradients on the development of a single or double-celled vortex and multiple vortices

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In this talk we show numerically the generation of single or double-celled vortices and multiple vortices in a cylinder non-homogeneously heated from below in a rotation frame. In a moderate rotation frame we show that the increase of thermal gradients is the responsible for the progression from a one-celled vortex, characterized by an updraft at the centerline, to a two-celled vortex, characterized by a central downdraft surrounded by updraft, i.e., a vortex that develops a central eye. If the thermal gradients continue increasing beyond a certain threshold, the axisymmetric eyed-vortex loses the axisymmetry, the eye displaces from the center and tilts. For larger rotation rates, the axisymmetric single-celled vortex does not progress to a double-celled vortex when the thermal gradients increase, but it becomes into a double vortex.

The change in the vortex type is also observed in laboratory tornadoes. In Ref. [1] it is shown the progression, as the swirl ratio increases, of vortex structure from a single cell to a two-cell vortex with a downdraft in the center. Our findings are relevant for their connection with the formation and evolution of some atmospheric vortices.

The numerical results have been obtained by direct numerical simulation of the time-dependent Navier-Stokes equations coupled with the heat equation, and the boundary conditions. These equations have been solved using a second-order time-splitting method proposed in Ref. [2], and described and tested in Ref. [3] for a cylindrical configuration. For the spatial discretization a pseudo-spectral method is used, with a Fourier expansion in the azimuthal coordinate ϕ and Chebyshev collocation in r and z.

Keywords: Vortices, Thermoconvective instabilities, Navier-Stokes equations
Acknowledgments. Partially supported by the Research Grants MTM2012-37642 MINECO (Spanish Government), which include RDEF funds, and GI20152914 (University of Castilla-La Mancha)

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Conjugated heat transfer simulation of a heated cylinder and an electronic device with the hybrid immersed boundary method

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In recent years the development of electronic devices has gone from increasing processor frequency and minimizing the size of the circuits to new methods to cool down the devices. For the moment the bottleneck lies in the cooling of both processors and memories. Especially for workstations, laptops, tablets and mobile phones that also need to be quiet and have a low external temperature. Fraunhofer-Chalmers research centre has developed a state-of-the-art flow solver called IPS IBOFlow [1]. The conjugated heat transfer module in IPS IBOFlow is developed to simulate cooling of electronic devices such as computers and mobile phones. The module handles fans, porous media, natural convection, IC resistors and thin thermal interfaces.

The solver is discretized on an adaptive octree grid and the presence of all objects are handled by the hybrid immersed boundary method [2, 3]. Hence, no boundary conforming grid is required and the mesh generation is automatic. To couple the solids with the octree background grid the solid volume fraction is calculated for each cell and face. In this work an approximate method is employed, where a least square plane is fitted to the cell-triangulation intersection. The resulting polygons and polyhedrons are employed to calculate the volume fractions. The solid heat transfer solver is also discretized on the octree grid, but it is only active in cells with non-zero solid volume fraction.

The solid solver is coupled to the fluid through heat fluxes, that are integrated over the local triangles. Finally, the fluid heat transfer solver is coupled with the solid solver through the hybrid immersed boundary method [4].

In this work the forced convection over a heated cylinder is simulated for a range of Reynolds numbers. The resulting Nusselt numbers are compared with experimental correlations and experiments. The comparison shows good agreement with experimental data. A grid convergence study is also performed, which shows that the relative error of the coupled solver converges with second order accuracy. Furthermore, to show the potential of the solver, the cooling of a small computer is simulated. A heat source of 50 W is added to the processor and the fan is cooling down the device. The resulting fluid and solid temperature distributions show how the processor is cooled down and other sensitive objects are heated up. Hence, the simulation predicts how the fan speed (applied voltage) can be adjusted such that the sensitive objects are not harmed.

Keywords: hybrid immersed boundary method, solid volume fraction, cooling of electronics.

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CT15: Model order reduction

Multirate-MOR for linear affine systems: Stability and error analysis

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The mathematic models of a multi-physics systems often lead to ordinary differential equations (ODE) with different dynamic properties: Some few components are changing very fast while the remaining ones are changing much slower. We consider linear affine systems of ODEs

$$\begin{pmatrix} \dot{w}_A(t) \\ \dot{w}_L(t) \end{pmatrix} = \begin{pmatrix} A_{AA} & A_{AL} \\ A_{LA} & A_{LL} \end{pmatrix} \begin{pmatrix} w_A(t) \\ w_L(t) \end{pmatrix} + \begin{pmatrix} g_A(t) \\ g_L(t) \end{pmatrix}$$

with $w_A(t), g_A(t) \in \mathbb{R}^{n_A},\ w_L(t), g_L(t) \in \mathbb{R}^{n_L}$ and a real system matrix A with corresponding dimensions. w_A includes all fast changing components and w_L all slow changing components. In practical application, it holds very often: $n_A \ll n_L$, that is only a few components are very active. Such systems fit well for time integration with multirate (MR) schemes that were introduced for multistep BDF methods in [3]: The slow changing subsystem is integrated with a large macro step-sizes H and the fast changing subsystem with smaller micro step-sizes h. To further reduce the numerical effort, a balanced-truncation model order reduction (MOR) is applied to the large, slow subsystem. The MOR causes a system error and the MR scheme a time integrations error:

$$E(t) = w(t) - \tilde{w}_n = \big(w(t) - \tilde{w}(t)\big) + \big(\tilde{w}(t) - \tilde{w}_n\big) = E_{MOR}(t) + E_{MR}(t)$$

with $w(t)$ the analytical solution, $\tilde{w}(t)$ the analytical solution of the coupled system with a reduced order, slow subsystem and $\tilde{w}_n$ the MR approximation of the coupled system with a reduced order, slow subsystem. For both errors there exist separate error bounds and stability condition, e.g. [2] for MOR and [1] for the MR θ-method. In [4] we showed how the combined error can be handled and bounded for linear systems. That includes a time domain error bound for coupled systems with order reduced subsystem. In this talk we will extend this work to the above given linear affine ODEs and give numerical results for the mathematical model of a benchmark system.

Keywords: Multirate time stepping, model reduction, coupled systems, balanced truncation.
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Parameterized model order reduction by superposition of locally reduced bases

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Modeling of scientific or industrial applications often yields high-dimensional dynamical systems due to techniques of computer-aided-design, for example. Thus a model order reduction is required to decrease the dimensionality to enable an efficient numerical simulation. In addition, methods of parameterized model order reduction (pMOR) shall preserve the physical parameters as independent variables in the reduced order models. We consider linear dynamical systems in the form of ordinary differential equations. In the domain of the parameters, often samples are chosen to construct a reduced order model. For each sample point a state-of-the-art method for model order reduction can be applied to compute a local basis. Moment matching techniques or balanced truncation schemes are feasible, for example, see [3].

A global basis for pMOR can be constructed from the local bases by a singular value decomposition (SVD), see [2]. However, the dimension of the global basis typically increases by extending the set of samples. The superposition of locally reduced dynamical systems was investigated in [5], where the strategy is similar to the trajectory piecewise linear approach for nonlinear model order reduction. We investigate a superposition approach that also takes only a few of the local models into account. Evaluating the reduced system in other than the sample points requires only an SVD of the closest local models' bases. Consequently for a fixed number of included local models the dimension of the reduced model is also bounded even if the number of sample points is increased. Our focus is on moment matching techniques using the Arnoldi procedure, see [4], and rational Krylov methods, see [1]. Hence the transfer function of the dynamical system is examined in the frequency domain. We present simulation results for a test example.

Keywords: parametric model order reduction, linear dynamical system, moment matching, singular value decomposition.

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CT16: Numerical methods in fluids

A self-adapting Local Projection-based solver for laminar and turbulent industrial flows.

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We address in this work the solution of the Navier-Stokes equations by Finite Element Local Projection Stabilization (LPS) methods. We focus on the high-order term-by-term stabilization method (*cf.* [1]). This method is a particular type of LPS scheme, which constitutes a low-cost, accurate solver for incompressible flows, despite being only weakly consistent. It differs from the standard LPS methods (*cf.* [2, 3]) because it uses continuous buffer functions, it does not need enriched FE spaces, it does not need element-wise projections satisfying suitable orthogonality properties, and it does not need multiple meshes. An interpolant-stabilized structure replaces the projection-stabilized structure of standard LPS methods. The interpolation operator takes its values in a continuous buffer space, different from the discrete velocity space, but defined on the same mesh, constituted by standard polynomials with one degree less than the FE space for the velocity. This approach gives rise to a method with reduced computational cost for some choices of the interpolation operator.

The interest of LPS methods is that the stabilization terms only act on the small scales of the flow. This ensures a self-adapting high accuracy in laminar regions of a turbulent flow, that turns to be of overall optimal high accuracy if the flow is fully laminar.

This also allows to obtain an asymptotic energy balance for smooth flows. We include some numerical tests that show that the solver accurately reproduces first-order and second-order statistics of benchmark turbulent flows.

Keywords: Turbulence modeling, local-projection stabilization, finite elements, high accuracy, asymptotic energy balance
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Stability of extrusion film casting process using a multimode PTT model

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Extrusion film casting (EFC) is a commercially important process that is used to produce several thousand tons of polymer films, sheets and coatings. The process consists of extruding a molten polymer through a center-fed "T" or a "coat-hanger" die under pressure; stretching the resulting molten film in air for a short distance (called as the take-up length, TUL) before being finally cooled down on a chill roll. In the present research, we focus on an extremely important instability that frequently occurs in high-speed EFC process known as draw resonance. Draw resonance manifests itself as periodic fluctuations in both the width as well as thickness of the extruded molten film. The phenomenon typically occurs above a critical draw ratio (DR) in spite of stable conditions of constant extruder throughput and chill-roll velocity. Studies on draw resonance phenomena have been done extensively in the past by several researchers. We refer in particular to the work of Silagy(Silagy et al 1996) and Zavinska (Zavinska et al 2008). These studies were done using a single mode viscoelastic constitutive equation. However, effect of multiple relaxation modes arising due to long chain branching polymer molecules on draw resonance has not yet been investigated. The aim of this work is twofold: First, to study the draw resonance instability on various Phan Than Tier (PTT) fluids as modeled by the parameter ϵ. Second, we aim to investigate the effect of multiple relaxation modes on the stability of EFC using a multi-mode PTT constitutive equation.The PTT equation is applied to each individual relaxation mode and the total stress is obtained by summation over the individual modes. Linear stability analysis is carried out by linearizing the mass, momentum and the stress equations and employing a modified Galerkin method to numerically calculate the eigenvalues of the linearized system. The simulations are done for a particular set of PTT model parameters. The stability diagrams show the stability regions for varying PTT model parmeter ϵ for different Deborah numbers (relaxation modes) and also for multiple Deborah numbers. The results show that for increasing values of the PTT model parameter the stability region shrinks. In the case of multiple modes, the effect of increasing number of relaxation modes is captured in the stability diagrams. Also, a comparison between the stability regimes of the multimode models and their corresponding averaged single mode model is performed. It is seen that there appears to be a marked variation in the two as the number of modes is increased indicating that caution needs to be exerted while representing a polymer with multiple relaxation modes by an averaged one. This kind of a complete stability map is important from a polymer processing perspective since it enables the selection of appropriate parameter and process conditions to stay in the region of stability.

Keywords: : extrusion, film, multi-mode, draw resonance, instability, relaxation modes, Deborah number
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A numerical approximation of a nonhydrostatic ocean model: first numerical results involving density driven flows

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Keywords: Navier-Stokes equations, nonhydrostatic ocean models, Lagrange-Galerkin, hp-finite element method, velocity-correction splitting.
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In the last decades ocean modelling has been carried out by models based on the hydrostatic primite equations of the ocean. It is well acepted that these models can properly describe important phenomena such as the wind-driven ocean gyres and the geostrophic eddies and rings. However, these models cannot resolve small scale phenomena (below 10 km) such as wind- and buoyancy-driven turbulence in the upper mixed layer, deep water convection or baroclinic instability; where nonhydrostatic models become essentials.

We present a numerical approximation of a nonhydrostatic ocean model. The nonhydrostatic models consist of the fully 3D Navier-Stokes equations formulated in a rotating framework for a fluid of variable density coupled with advection–diffusion equations for temperature and salinity plus the equation of state for the density. To deal with the advection terms the Lagrange-Galerkin method is chosen that yields symmetric and well conditioned problems for the advection-diffusion equations for temperature and salinity and a Stokes-like problem for the Navier-Stokes equations. The latter is discretized by a velocity-correction splitting that separates the calculation of the velocity and pressure. Furthermore, the pressure is decomposed into hydrostatic and nonhydrostatic component. Regarding the spatial discretization, hp-finite element method is used.

Many important phenomena in oceans such as internal wave formation, deep water convection, slope bottom currents or water interchange through straits are based on strong density differences in the flow. We show the efficiency of the proposed numerical approach in several simulations of density driven flows.

CT17: Numerical algebra
Numerical integration

Approximating a class of nonlinear fourth-order ordinary differential problems

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Differential matrix models are an important component of many interesting applications in science and engineering. This work elaborates a procedure to approximate the solutions of special nonlinear fourth-order matrix differential problems of the type

$$Y^{(4)}(x) = f\big(x, Y(x)\big), \quad x \in [a, b],$$

by suitable matrix splines [1]. Traditionally, the scalar fourth-order ordinary differential equations are transformed to a first-order system of ordinary differential equations so that standard numerical methods may be applied. However, this technique comes with an increase of computational cost due to the higher dimensionality of the problem. For this reason, in the scalar case, direct integration methods have attracted significant attention for solving fourth-order or higher-order problems. These direct methods give impressive advantages in accuracy and speed over the conventional approach, see [2, 3, 4] and references therein, which we now generalize to matrix systems. In conclusion, we provide two examples of the proposed matrix method and demonstrate its efficiency.

Keywords: Higher-order matrix splines, fourth-order matrix differential equations.
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An application of the hyperfunction theory to numerical integration

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In this study, we examine a numerical integration method proposed by Hirayama [1] theoretically and numerically, and refer to its relation with the hyperfunction theory, a theory of generalized functions proposed by Sato [2, 3]. Let $\int_a^b f(x)w(x)\mathrm{d}x$ be the integral of a given function $f(x)$, which is assumed to be analytic in a neighborhood domain D of the interval $[a,b]$, with a weight function $w(x)$. In Hirayama's method, we transform the desired integral by the Cauchy integral formula into the complex contour integral

$$\int_a^b f(x)w(x)\mathrm{d}x = \frac{1}{2\pi\mathrm{i}}\oint_C f(z)\Psi(z)\mathrm{d}z \quad \text{with} \quad \Psi(z) = \int_a^b \frac{w(x)}{z-x}\mathrm{d}x, \tag{0.1}$$

where C is a closed path encircling the interval $[a,b]$ in the positive sense and included in the domain D, and compute the integral by approximating the complex integral on the right-hand side of the first equation in (0.1) by the trapezoidal rule. The analytical forms of the functions $\Psi(z)$ are known for some typical cases. This method works very well since the trapezoidal rule is efficient especially for the integral of a periodic analytic function over a one-period interval. In fact, a theoretical error estimate shows the geometric convergence of the approximation of the method and numerical examples show that the method is efficient especially for integrals with strong end-point singularities.

We mention the relation between Hirayama's method and the hyperfunction theory. Roughly speaking, a hyperfunction $f(x)$ on an interval (a,b) is the difference of the boundary values of an analytic function $F(z)$ as $f(x) = F(x+\mathrm{i}0) - F(x-\mathrm{i}0)$. Here, $F(z)$ is called the defining function of the hyperfunction $f(x)$ and is analytic in $D \setminus [a,b]$, where D is a neighborhood domain of $[a,b]$. The integral of the hyperfunction $f(x)$ on the interval $[a,b]$ is defined by $\int_a^b f(x)\mathrm{d}x = -\oint_C F(z)\mathrm{d}z$, where C is a closed path encircling $[a,b]$ in the positive sense and included in D. In Hirayama's method, the integrand $f(x)w(x)$ of the desired function can be regarded as a hyperfunction whose defining function is $-1/(2\pi\mathrm{i})f(z)\Psi(z)$, and we compute the integral by approximating the complex integral which defines the integral of the hyperfunction $f(x)w(x)$.

In this study, we also extend Hirayama's method to integrals over infinite intervals and Hadamard's finite part integrals.

Keywords: numerical integration, hyperfunction, complex integral
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Symplectic Lancozs method for solving linear hamiltonian systems of ODEs

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Krylov subspace methods have become popular for the numerical approximation of matrix functions as for example for the numerical solution of large and sparse linear systems of ordinary differential equations. One well known technique is based on the method of Arnoldi which computes an orthonormal basis of the Krylov subspace [3]. However, when applied to Hamiltonian linear systems of ODEs, this method fails to preserve the symplecticity of the solution under numerical discretization, or to preserve energy. In this work we apply the Symplectic Lanczos Method to construct a J-orthogonal basis of the Krylov subspace. Following ideas from [4], this basis is then used to construct the numerical approximation. The resulting projected problem is a Hamiltonian system of smaller size and the approximation produced is energy-preserving.

The symplectic Lanczos method is widely used to approximate eigenvalues of large and sparse Hamiltonian matrices [1]. In this context a number of techniques for the restart of the algorithms have been proposed in the literature. The approach for solving linear Hamiltonian systems is less well known. We here consider a technique to restart the iterations when applying the Symplectic Lanczos methods. This approach is similar to what is used in classical Krylov projection methods for systems of ODEs [2]. We analyse the geometric properties and the growth of the global error as a function of time for both the methods.

Keywords: hamiltonian, symplectic, projection, sparse matrices.

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CT18: Finite differences

Modelling of combustion and diverse blow-up regimes in a spherical shell

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The second-order nonlinear parabolic equation has proved to be an adequate model for describing many evolutionary processes in plasma physics, chemical kinetics, biophysics, IT, social sciences etc. [1, 2, 4, 7]. It is especially useful for modelling regimes with blow-up that occur in open dissipative nonlinear systems with positive feedbacks. While the nonlinear diffusion term allows simulating dissipative processes in the system, the external forcing is aimed to model cumulative processes. The accumulation and dissipation are the key components of the dynamics of complex systems, and their unity is the driving force of evolution.

A particular interest of the present work is the phenomenon of combustion and its different critical blow-up regimes resulted from a drastic increase of the temperature within a bounded region for a finite time. We consider a 3D nonlinear diffusion model in a spherical shell. To solve it numerically, we split the differential operator along the radial coordinate, as well as involve an original technique of using two coordinate maps for solving the 2D subproblem on the sphere. Hence, eventually we have to solve two 1D finite difference problems with simple periodic boundary conditions in the latitudinal and longitudinal directions respectively that lead to unconditionally stable implicit second-order finite difference schemes. A band structure of the resulting matrices allows applying fast direct (non-iterative) linear solvers using the Sherman-Morrison formula and Thomas algorithm [6]. We test the developed method in several series of numerical experiments aimed to study three critical regimes of combustion caused by a nonlinear term in the source function: the HS-regime of combustion in an expanding area, the LS-regime of combustion in a reducing area and the S-regime of combustion in a fixed-size area. In all the regimes a blow-up occurs due to a violent growth of the temperature within a finite time.

This study is an extension of our previous work in which we considered two-dimensional combustion on a sphere [8]. The new results demonstrate that a three-dimensional nonlinear parabolic equation allows modelling different regimes of combustion in a 3D complex domain. The heat localisation is shown to lead to the breakup of the medium into individual fragments followed by the formation and development of self-organising patterns [3, 4, 7], which may have promising applications in thermonuclear fusion [4], nonlinear inelastic deformation and fracture of loaded solids and media [5] and other areas.

Keywords: Nonlinear parabolic equation, localised blow-up in complex media, patterns formation and self-organisation, finite difference schemes, operator splitting.
Acknowledgments. This work was partially supported by the research grant No. 14539 of the National System of Researchers of Mexico (SNI, CONACYT).

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Non–local linear filtering for advanced remote sensing applied to surface coal mining affected areas mapping

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Surface coal mining activities led in the past to serious land cover damages. Accurate estimation of affected areas dimensions is a key point, e.g. for latter environmental restoration. To this end remote sensed data turned out to be from several years ago a very helpful tool to classify each area as affected or non–affected. However, it has been reported that most of commonly used classification methodologies are affected for several sources of noise: adverse atmospheric conditions, a great variety of vegetation, isolated reflectance spots, small size affected areas, and so on.

Our main contribution lies in the use, among an unsupervised classifier, of a non–local filter at the pre–classification stage, and a convenient re–classification methodology at the post–classification stage. A first approach to pre–processing by means of non–local filtering was successfully studied in [3, 4], in this occasion to estimate forest fires affected areas and by using filters of fractional type.

The mathematical model we set is a finite dimensional (in space) non–local linear evolution equation

$$(1) \quad \partial_t \mathbf{u}(t) = \mathbf{u}_0 + \int_0^t \mathbf{K}(t-s)\mathbf{u}(t)\,\mathrm{d}s, \quad 0 \le t \le T,$$

where $\mathbf{u}(t)$ represents the image at time level t evaluated on a uniform mesh of a square domain Ω vector arranged; $\mathbf{u_0}$ stands for the original input; ∂_t stands for the time derivative; and $\mathbf{K}(t)$ is a given matrix–valued convolution kernel. Typically, a convenient numerical discretization of (1) reads

$$(2) \quad \mathbf{u}_n = \mathbf{u}_0 + \sum_{j=0}^{n} \mathbf{K}_{n-j}\mathbf{u}_j, \quad 0 \le n \le N,$$

where $\mathbf{K}_n$, for $0 \le n \le N$, depends on the step–size of the time discretization, i.e. $h = T/N$, and $\mathbf{u}_n$ stands for the approximation to $\mathbf{u}(t_n)$ where $t_n = nh$.

Numerical experiments over several areas located in the northern Spain will be shown, and different criteria to measure the efficiency of our methodology and the five indexes we chosen for our study, obtained from Landsat 8 Operational Land Imager data or determined in terms of these, will be discussed.

Keywords: Remote sensing, non–local filtering, coal mining, land cover.

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Numerical solution of a 2D multispecies biofilm model based on PDEs

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A biofilm mainly consists of a layer of prokaryotic and eukaryotic cells anchored to a substratum surface. This layer is embedded in a EPS matrix, that keeps bacteria tied and makes difficult their removal. Sometimes biofilms have negative impact in medicine, environment and food industry, giving rise to pollution or infections. However, in other cases they have positive effects, such as in water treatment plants [1]. In our case, the main motivation comes from the interest of IIM-CSIC in a suitable modelling of biofilms and its efficient numerical simulation to characterize *Listeria monocytogenes* bacteria appearing in food industry.

In recent years many numerical models have been developed, specially stochastic ones. Our work focuses on the numerical solution of a continuum model in order to apply it to the characterisation of the evolution and growth of the Listeria bacteria. In a previous work, we studied a single species model considering only the evolution of active biomass [5]. Our current study is mainly based on the model presented in [2], a system of nonlinear diffusion-reaction parabolic equations that governs the evolution of the active and inert biomass limited by the amount of oxygen available.

In order to solve the model, we use efficient numerical methods, particularly upwind finite differences methods modified as described in [3], a level set method [4], WENO schemes, TVD-RK numerical techniques and a Newthon-Raphson algorithm for the nonlinear system of discretized equations. Also, the set of numerical methods has been implemented as an efficient C++ code.

Finally, we will present some illustrative examples of the numerical solution. Our results show that the model is able to qualitatively represent the biofilm behavior, the level set method being a fundamental numerical technique, due to the efficiency it adds to the code and the consequent simplifications to solve the PDE system, thus avoiding to solve the discretized system in the whole domain at each iteration.

Keywords: Biofilms, Nonlinear partial differential equations, Finite differences, Level Set Methods.
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CT19: Other mathematical topics and their applications

Fast ray tracing on phase space for optical systems

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Ray tracing is a widely used method in optical design to calculate photometric variables at a target. Given an optical system a set of rays is traced from the source to the target. For each ray both the initial position and the angle with respect to the normal of the optical axis are given. Each time that a ray hits an optical surface (lens or reflector), the position on the surface and the new direction of the ray are calculated. The calculation stops when the ray reaches the target. To compute the target distribution, the procedure is repeated for a large sample of rays. In non-imaging optics the most commonly used ray tracing process is Monte Carlo (MC) ray tracing [1] which is based on a probabilistic interpretation of the ray distribution at the source. The rays are traced randomly and, the photometric variables are implemented partitioning the target into so-called bins and considering the number of rays that fall into each of these bins. As a consequence, millions of rays are required to obtain a reliable result. Therefore, the technique is very slow and converges as the inverse of the square root of the number of rays traced.

We propose a new ray tracing technique to speed up the method. Our procedure is based on the phase space (PS) representation of the source and target, where each ray is described by its position and its angle with respect to the optical axis. In addition, the algorithm computes the sequence of the optical surfaces that each ray hits when it propagates through the system. We use this information to describe the ray distribution at source and target PS, which can be partitioned in different regions according to the path followed. Assuming constant brightness, we only need to compute the boundaries of these ray sets to obtain the photometric variables at the target. Two different methods to compute the boundaries of these regions are provided. The first method is based on the α-shape of the point cloud given by the rays on PS. Given a triangulation of the point cloud, the corresponding α-shape is the union of all the triangles having a circumcircle of radius smaller than α. The α-shapes method strongly depends on the value of the parameter α and, it is difficult to estimate the value that provides the best approximation of the boundaries. Thus, a more accurate procedure to compute the boundaries is needed. For the alternative method, the boundaries at the source PS are calculated and, employing the edge-ray principle [2], also the target boundaries are determined. To do this, an adaptive triangulation of the source PS is constructed such that new triangles are added only where boundaries occur. The triangulation is based on the fact that a boundary is expected between two rays that follow different paths. Two different criteria to stop the refinement procedure are considered. For the first criterion, the rays traced must follow the same path; for the second, they have to be located close to each other in PS.

Ray tracing is a general technique applicable to any optical system; we developed a numerical algorithm to simulate ray tracing for a two-dimensional Total Internal Reflection (TIR) collimator. The error between the approximate intensity and the reference intensity is computed both for MC and PS ray tracing. Numerical results show that the PS approach is much faster and more accurate than the already existing ray tracing methods and converges as one over the number of rays traced.

Keywords: Ray tracing, Monte Carlo ray tracing, phase space, optical systems, TIR-collimator.
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Gibbs tessellations and foam modeling

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The microstructure of cellular materials, especially foams, may be characterized by the length of the edges and the shape of the cells, which can be estimated from e.g. computertomographic images. The common modeling techniques are based on Laguerre tessellations generated by a parametric point process (e.g. a sphere packing, see [1]). They are able to reproduce the distribution of the size of the cells and at most the shape of the cells, but not the typical edge-length distribution (see [2]). We use a different approach - Gibbs tessellations (see [3]) - including the geometric characteristics of the tessellation in the density. With this intuitive approach we make direct use of properties of the cells and do not need to use the generating points in the model, a major difference to common models.

A variety of geometric properties of the cells or the tessellation can be considered which leads to a wide field of possible densities. Exemplary models for isotropic and anisotropic foams will be presented. Additional remarks on the computational and mathematical background of this model complete the talk.

Keywords: Material Characterization, Gibbs Processes, Spatial Statistics, Stochastic Geometry, Monte Carlo
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Prototype model of autonomous offshore drilling complex.

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The perspective way of oil and gas field development in the Arctic region is construction of autonomous drilling complexes that are mounted on the seabed and don't have direct connection to the sea surface. The technical specifications of such devices also imply the exploitation below the sheet of ice that makes them universal and independent from weather and ice conditions

Presently this technology is still inelaborate and has no comparable counterparts. The prototype modelling is extensively used on this stage of development. The main objectives of prototype modelling are the specification of the requirements to drilling complex and design verification by performing of multiple virtual tests of the system and its components.

The prototype model of autonomous offshore drilling complex consists of several sub models corresponding to different considered phenomena: vibrations of drilling string; circulation of drilling mud; mud filtration; deformation of the liquid filled soil and so on. All sub models are combined into unified prototype model and exchange data during simulations.

The project of prototype model development is launched jointly by St. Petersburg Polytechnic University and Rubin ship design bureau. Both commercial and in house software are used for simulation by applying methods from different branches of computational mechanics.

Keywords: prototype model, computational mechanics, offshore drilling complex

Travelling waves in Smectic C^* crystals with anisotropy

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We consider travelling wave solutions for a smectic C^* liquid crystal system [3] subject to an electric field, which involves analysing a quasilinear parabolic equation governing the dynamics of te director $\phi(x,t)$,

$$\phi_t = ([1-\xi\cos(2\phi)]\phi_x)_x - \xi\sin(2\phi)\phi_x^2 - \frac{d\hat{w}}{d\phi}, \tag{0.1}$$

where ξ measures elastic anisotropy and the free energy density $\hat{w}$ is given by

$$\hat{w}(\phi) = \frac{1}{2}\sin\phi + \frac{1}{4}\beta\cos^2\phi, \tag{0.2}$$

with β proportional to dielectric anisotropy and the magnitude of the applied electric field. We use the variational methods of Benguria and Dupassier [1] and the criteria for the realisation of linear and nonlinear selection mechanisms derived in [2] to understand the the effect of anisotropy on the minimal speed of the travelling wave.

Keywords: Smectic C^* liquid crystals, anisotropy, travelling waves, variational methods, selection criteria.

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Independent loops search in flow networks aiming for well-conditioned system of equations

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In both mesh-current analysis and pipeflow analysis it is required that one can find a set of independent loops in order to obtain a well-defined set of equations for the unknown variables. In mesh-current analysis the unknown variables are the loop currents, and in pipeflow analysis the unknowns are flow rates in the pipes. In terms of graph theory, the problem of finding such independent loops is equivalent to finding a set of circuits such that the circuits are linearly independent under the ring sum operation.

In mesh-current analysis the independent loops result in a linear set of equations according to Kirchhoff's voltage law, whereas in pipeflow analysis the corresponding set has both linear and nonlinear equations with respect to the flow rates. The linear equations correspond to continuity of flow, i.e., for each node flow in equals flow out, and the nonlinear equations correspond to head loss over any closed loop equaling zero. However, the nonlinear equations can be linearized and solved iteratively as described in [4].

Especially in the context of mesh-current analysis, different methods have been proposed to determine the independent loops, e.g., [1] and [2]. Furthermore, a set of independent loops can be found using the concept of fundamental circuits of graph theory [3]. However, even though a number of different methods exists for finding these independent loops, very little emphasis is put on considering how well-conditioned the resulting set of linear(ized) equations will be. This aspect is especially important in the case of pipeflow analysis where any loss of numerical accuracy in solving the linearized equations carries over to the next iteration, and at worst case, causes the iterations to diverge.

We will consider constructing the independent loops using various methods and inspect the condition numbers of the matrices corresponding to the obtained set of linear(ized) equations. Furthermore, we will present techniques for enhancing the condition number of the resulting matrices as well as give ideas on how the condition number of a matrix can be affected in general. The presented techniques and ideas will be demonstrated on test cases arising from pipeflow analysis.

Keywords: linear equations, graph theory, pipeflow analysis, circuit analysis, independent loops.
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Cosimulation convergence criteria for coupled implicit DAEs of index 2

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The network approach to the modelling of complex technical systems results frequently in a set of coupled differential-algebraic equations (DAEs). Dynamic iteration methods, also referred to as cosimulation or waveform relaxation methods, are well-established since they allow for dedicated solvers and discretization grids for the involved subsystems. Unlike ordinary differential equations (ODEs), coupled DAE-systems may suffer from instability during a dynamic iteration. This article presents a convergence criterion for coupled systems involving semilinear implicit DAEs of index 2. Furthermore, for the application field of electrical circuits, it is shown how this criterion can be checked by means of the topology of the circuit.

Keywords: Cosimulation, Dynamic Iteration, DAEs, index 2, implicit, semilinear, Convergence Criterion, Contraction.
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