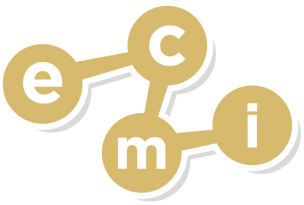
20^{th} European Conference on Mathematics for Industry

June, 18-22, 2018, Budapest (Hungary)



BUDAPEST 2018

EUROPEAN CONSORTIUM FOR
MATHEMATICS IN INDUSTRY

Book of Abstracts

EDITED BY Ágnes Bodó, Imre Fekete, Ferenc Izsák, Gábor Maros, Péter L. Simon

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Welcome at ECMI 2018

On behalf of the Organizing Committee, we are pleased to welcome you in Budapest for the 20th European Conference on Mathematics for Industry, ECMI 2018.
We are thankful and proud for being selected to host this special anniversary. Hungary is well-known for its outstanding achievements in pure mathematics, but much less known for its contributions to applied mathematics, in spite of the works of outstanding scientists like, Gyula Farkas, Theodore von Kármán, John von Neumann or Rudolf E. Kalman. Therefore it is our privilege to have the opportunity to reinforce our contacts with the major European network promoting industrial mathematics, by bringing together more than 350 researchers for intellectual interaction for 5 days.

The European Consortium for Mathematics in Industry (ECMI) organized its first international conference in Oberwolfach, in 1983, followed by a series of conferences, a persistent objective of which has been to galvanize interaction between academy and industry, leading to innovations in both fields. We hope that ECMI 2018 will further inspire multidisciplinary research along these lines, leading to the formulation of real-life challenges, where mathematical technologies may provide significant new insights.

Following the traditions of ECMI, the conference will focus on various fields of industrial and applied mathematics, such as Applied Physics, Biology and Medicine, Cybersecurity, Data Science, Economy, Finance and Insurance, Energy, Production Systems, Social Challenges, Vehicles and Transportation. These themes nicely fit to current distinguished national research programs in Hungary, in particular programs on Autonomous Vehicles, Digital Factories, Brain Research or Precision Agriculture, supported by the EU and the National Research, Development and Innovation Office.

The conference is jointly organized by the János Bolyai Mathematical Society, the Institute of Mathematics at Eötvös Loránd University, and the Institute for Computer Science and Control of the Hungarian Academy of Sciences (MTA SZTAKI). The newly appointed Minister of Innovation and Technology, László Palkovics was kind enough to patronize our conference.

The statistics of the conference are more than satisfactory. In addition to the nine plenary talks, given by world class researchers, we have 50 minisymposia, and 45 contributed talks and poster presentations, running in 7 parallel sessions. Altogether we have more than 350 participants, from around 40 countries. More than 50 participants are students.

We express our deepest gratitude to everybody involved in the preparation of this meeting, the plenary speakers, the members of the Scientific Committee, the organizers of the minisymposia, the contributing authors and all the participants of the conference.

It is our pleasure to acknowledge the financial support of Graphisoft, Secudit, Morgan Stanley, and the EPIC Centre of MTA SZTAKI, providing the financial basis for the participation of many young researchers. We recommend that you take time for exploring the beauty of our capital, but first of all we wish to all of you an intellectually stimulating, successful conference.

Budapest, June 2018

On behalf of the Organizing Committee

Péter L. Simon (chair), László Gerencsér (advisor), Ferenc Izsák (secretary)

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Plenary talks

Traffic Managment by Macroscopic Models

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Macroscopic traffic flow models have become popular in transportation engineering and applied mathematics during the last decades. These models give a description of collective dynamics in terms of spatial density and average velocity, which evolve according to partial differential equations derived from fluid dynamics, coupled with suitable closure relations. In fact, even if the continuum hypothesis is clearly not physically satisfied, macroscopic quantities can be regarded as measures of traffic conditions and allow depicting the spatio-temporal evolution of traffic waves. Moreover, they are suitable for analytical investigations and very efficient from the numerical point of view. Therefore, they provide the right framework to state and solve control and optimization problems for real time applications.

Starting from the celebrated Lighthill-Whitham-Richards model [6, 10] formulated in the mid 50ties, mathematicians and engineers designed various more sophisticated models in order to capture specific traffic characteristics. These include second order [1**?**], phase-transition [3] and non-local models [2]. Extensions to road networks have also been addressed by providing suitable models describing the dynamics at junctions [4]. These improved models are expected to better match observations based on real data coming form different sources: besides the traditional magnetic loop detectors, the recent technological developments provide data extracted from video recording, GPS, Bluetooth, RFID, etc.

In my talk, I will briefly review the basis of the macroscopic approach for modeling vehicular traffic, and I will show how these models can be efficiently implemented for traffic flow optimization. In particular, I will focus on traffic control strategies based on ramp-metering [9], variable speed limits [5] and partial rerouting [11]. Further control perspectives are offered by the future deployment of autonomous vehicles [8].

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Div Grad Curl are Dead - Are they?

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Being inspired by the title of Burke's unpublished book [1] we ask ourselves: What is the future role of physics-based modeling, simulation and optimization (MSO) in the age of machine learning (ML) and artificial intelligence (AI)? As a matter of fact, the use of simulation has seen continual double digit percentage growth annually for about 30 years until 2008.

To continue this success story during the next decade, MSO needs to become *"increasingly fit for purpose, smart, integrated, and transparent"* (Joe Walsh, NAFEMS2015). Mathematical key technologies to enable such progress will be highlighted in this talk.

We start by considering industry: what is the role of mathematics and what are topical needs? Sustaining Moore's law necessitates parallel computing. For example, multi-objective optimization with evolutionary algorithms is embarassingly parallel. The computation of eddy current losses in the winding heads of electrical machines by large-scale high performance computing serves as another example.

Along with Moore's law in hardware goes a similar evolution of algorithms. Multi-domain, multi-scale and multi-fidelity simulations, in short multi-X, are coming within reach now, with powerful simulation frameworks. We demonstrate this for quench propagation in superconducting accelerator magnets [2], by employing the port-Hamiltonian approach. We also discuss the co-evolution of Computer-Aided Design and Finite-Element Analysis into Isogeometric Analysis. This makes the exact geometry accessible for numerical analysis, for example for computing resonant electromagnetic modes in superconducting accelerator cavities [3].

We conclude that data-driven models based on ML and AI will not render physical domain-specific models obsolete. In contrast, both model classes complement each other very well in hybrid approaches. Div, Grad, Curl will be going stronger than ever!

Acknowledgments The author is grateful to Bernhard Auchmann (CERN, Geneva), David Morisco, Oliver Rain (both Robert Bosch GmbH), and Sebastian Schöps (Graduate School Computational Engineering, TU Darmstadt).

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Modelling CO_2 Storage in Large-scale Aquifer Systems

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Large-scale storage of CO_2 in saline aquifers is considered an essential technology to mitigate carbon emissions. The injected CO_2 will form a buoyant plume that can migrate long distances as a thin sheet under a sloping impermeable caprock. The plume migration can be described by mass conservation of CO_2 and brine, which together with Darcy's law form a mixed elliptic-hyperbolic system of PDEs. Solving this system with the accuracy required to track the plume movement over thousands of years is rarely computationally tractable. In the talk, I present suitable model simplifications.

The simplest possible model to estimate storage capacity assumes infinitesimal flow rates and uses geometrical analysis of the caprock topography to determine catchment areas, spill paths, and structural traps. As a mental picture, you can think of water trickling down a terrain to form ponds, rivers, and lakes. The next type of model assumes that vertical fluid equilibrium is reached instantaneously. Integrating the 3D model equations vertically, one obtains a 2D semi-analytical, elliptic-parabolic problem posed over a surface grid. This not only reduces the required number of grid cells, but also improves time constants significantly. If needed, one can form multilayered models and/or use a combination of depth-integrated and 3D models in different parts of the aquifer.

In the last part of the talk, I discuss how to mathematically optimize the placement of injection points and their fluid rates to maximize storage while minimizing the risk of CO_2 leaking back to the surface. This includes use of adjoint formulations and simplified forecasts of migration paths for early termination of the forward simulations.

Acknowledgments The author is grateful for the support from the Norwegian CCS Research Center.

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Heterogeneity in Acute Leukemias and its Clinical Relevance: Insights from Mathematical Modelling

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In this talk I present a mathematical approach to understand dynamics of acute leukemias which are among most frequent hematopoietic malignancies. A hallmark of acute leukemias is clinical heterogeneity, i.e., inter-patient differences in the disease dynamics and response to therapy. Moreover, recent sequencing studies show that the population of leukemic cells exhibit intercellular heterogeneity. Genetic and phenotypic interdependence of the different clones is complex and so far not well-understood. We propose a range of mathematical models describing evolution of a multiclonal and hierarchical cell population to investigate the impact of mutation and selection on the course of the disease. In particular, the models in form of differential and integro-differential equations are applied to study the role of stem cell properties and regulatory feedbacks in emergence and evolution of clonal heterogeneity. It is shown how resulting nonlinear and nonlocal terms may lead to a selection process and ultimately to therapy resistance. The results help to understand which phenotypes may be present at different times over the course of disease and how treatment affects the clonal evolution of the disease. Model-based interpretation of clinical data of individual patients allows estimating parameters that cannot be measured directly. This may have clinical implications for future treatment and follow-up strategies.

Hybridized Discontinuous Galerkin and Model Order Reduction Methods with Applications to Health and Physics

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I created the Center for Modeling and Simulation of Strasbourg (Cemosis) in 2013 with the objective to develop the mathematics at the interface with other disciplines, enterprises, and society. We decided back then to have an approach to research which was application driven, interdisciplinary and collaborative. In this context, we have developed national and international partnerships in health and physics where modeling, simulation, optimization (MSO), high-performance computing, data science are core components. In our strategy, software development plays a crucial role, it is, with the joint publications, the glue in our collaborations. To this end, we have developed a framework called Feel++ for solving partial differential equations (PDE) using a broad range of Galerkin methods.

In this talk, I am going to present recent contributions to hybridized discontinuous Galerkin (hdG) methods as well as model order reduction methods which were integrated into Feel++. These contributions have been developed to solve bottlenecks in our applications. I start with hdG in the context of PDE with integral boundary conditions often involving the coupling with a 0D model [1]. I present the mathematical and computational frameworks as well as numerical results and applications. The coupling strategy in the presence of 0D models is also discussed. Then I show our recent contributions in reduced order methods [2] as well as new results, namely the reduced basis method (RBM) and the empirical interpolation methods (EIM), and in particular in using them to solve non-linear multi-physics PDE with an affordable cost. Until recently, these methods were too prohibitive to be considered in industrial applications involving non-linear multi-physics PDE solves. I will illustrate these findings with two of our flagship applications at Cemosis, Eye2brain(Health) and Hifimagnet(Physics), which are going to be further demonstrated in the mini-symposium MS21 of ECMI 2018.

Acknowledgments This work would not have been possible without the contributions of many collaborators in France, in Italy and the USA on our projects at Cemosis. This work has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 731063 as well as the French National Research Agency program under the grant Chorus and the LabEx IRMIA.

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Three-dimensional X-ray Vision by Sparse Tomography

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Traditional X-ray tomography is used routinely in hospital CAT-scans and in industrial non-destructive testing. There the idea is to collect a large number of X-ray projection images from all around the object, interpret the data as line integrals over a non-negative X-ray attenuation coefficient function, and reconstruct the inner structure of the target. Typically, the reconstruction algorithm of choice is some variant of Filtered Back-Projection (FBP). However, in many practical applications there are radiation dose restrictions or geometric obstacles preventing the collection of a comprehensive dataset. In such cases the FBP algorithm does not perform optimally. In recent years there has been tremendous progress in the development of robust reconstruction algorithms for sparse-data tomography. One of the successful approaches is variational regularization with a sparsity constraint; this approach is closely related to compressed sensing. In the talk, examples of sparse-data tomography are presented from the fields of dental imaging, biomedical specimen analysis, and detecting defects in weldings.

Acknowledgments The author is grateful for the support of TEKES (grant 6614/31/2016) and the Academy of Finland (Academy project 310822, Centre of Excellence in Inverse Problems Research 2012–2017, decision number 250215, and Centre of Excellence in Inverse Modelling and Imaging 2018–2025, decision number 312339).

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Hardware-in-the-loop Experiments on Bistability

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A widely used tool of engineering research and development is the hardware-in-the-loop (HIL) experiment. Instead of building the full prototype of a developed machine, only its most critical parts are constructed physically, while the rest of the machine is emulated by means of actuators, sensors, and digital control in between. If the mathematical model of the rest of the machine is available, the control unit can provide a realistic environment for the physically constructed test part. The control, however, introduces digital effects into this system which is originally continuous. From dynamical view-point, the most relevant digital effects are the appearances of delay and zero-order-hold (ZOH). The nonlinear dynamics of the real system and the one constructed by means of the HIL experiment are compared from stability and nonlinear vibrations view-point in case of a brake system where stick-slip phenomenon occurs. The limitations of HIL experiments are identified by means of Hopf bifurcation calculations, numerical simulations and dynamic measurements carried out on the corresponding experimental test rig. The results then applied for the development of HIL experiments on high-speed-milling (HSM).

The Legacy of Rudolph Kalman

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In 1960 Rudolph Kalman published what is arguably the first paper to develop a systematic, principled approach to the use of data to improve the predictive capability of the mathematical models humans have developed to understand the world around us. As our ability to gather data grows at an enormous rate, the importance of this work continues to grow too. The lecture will describe this paper and developments that have stemmed from it, revolutionizing fields such space-craft control, weather prediction, oceanography, oil recovery, medical imaging and artificial intelligence. Some mathematical details will be also provided, but limited to simple concepts such as optimization and iteration; the talk is designed to be broadly accessible to anyone with an interest in quantitative science.

Minisymposia

MS 01: Fractional diffusion: modeling, theory and numerics

Umbral Fractional Calculus and Applications

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Different problems in applied science require novel mathematical methods to get more general solutions amenable for a wider applicability using advanced computational tools [1].

Fractional derivatives are getting increasing attention to deal with problems in Social Sciences, Biology, Mathematics, Physics...

Within such a context, the use of fractional PDE is a wide spread tool to model non classical diffusion problems, occurling in Economy, Plasma Physics, non equilibrium Termo-dynamics, just to quote a few examples. The mathematical language underlying the fractional calculus has undergone a spectacular evolution during the last decade. Many aspects of the relevant theory need to be clarified.

In this contribution we discuss a number of problems and of practical recipes concerning the solution of fractional PDE including the associated ordering problems which, albeit extremily important, did not receive an appropriate treatment so far. We will show how a very effective tool is the use of Umbral type methods to merge fractional and pseudo differential operators.

We will finally discuss specific problems including applications for the diffusion problems, Laser physics and fractional Poisson processes [2, 3].

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Numerical Solution of Nonstationary Problems for a Space-fractional Diffusion Equation

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Many applied mathematical models involve both sub-diffusion (fractional in time) and super-diffusion (fractional in space) operators. Super-diffusion problems are treated as evolutionary problems with a fractional power of an elliptic operator. For example, suppose that in a bounded domain Ω on the set of functions $u(\mathbf{x}) = 0,\ \mathbf{x} \in \partial\Omega$, there is defined the operator $\mathcal{A}$: $\mathcal{A}u = -\triangle u,\ \mathbf{x} \in \Omega$. We seek the solution of the Cauchy problem for the equation with the fractional power elliptic operator:

$$\frac{du}{dt} + \mathcal{A}^{\alpha} u = f(t), \quad 0 < \alpha < 1, \quad 0 < t \leq T,$$

$$u(0) = u_0,$$

for a given $f(\mathbf{x}, t)$, $u_0(\mathbf{x}),\ \mathbf{x} \in \Omega$ using the notation $f(t) = f(\cdot, t)$.

Standard two-level schemes are applied to solve numerically a Cauchy problem for an evolutionary equation of first order with a fractional power of the operator. The numerical implementation is based on the rational approximation of the operator at a new time-level. When implementing the explicit scheme, the fractional power of the operator is approximated on the basis of Gauss-Jacobi quadrature formulas for the corresponding integral representation. In this case, we have a Pade-type approximation of the power function with a fractional exponent. A similar approach is used when considering implicit schemes.

On the Use of Fractional Derivatives in Fluid Dynamics Simulations

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Computational Fluid Dynamics is one of the most researched and most innovative field of computational mathematics. The fundamental basis of almost all CFD problems is the Navier–Stokes equations.

The Navier–Stokes equations for the velocity field $\mathbf{u} : \Omega \to \mathbb{R}^2$ and the pressure function $p : \Omega \to \mathbb{R}$ of an incompressible fluid are given as

$$\begin{aligned} (-\mathbf{u} \cdot \nabla)\mathbf{u} - \nabla p + \nu \Delta \mathbf{u} &= 0 \\ \nabla \cdot \mathbf{u} &= 0. \end{aligned} \tag{1}$$

In this talk we present an iteration technique based on fractional derivatives to solve (2) numerically summarizing our work [1] . We also prove the convergence of the corresponding iteration. The method is tested on different benchmark problems and the simulation results are in a good accordance with real measurements.

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An Efficient Numerical Simulation of Space-Fractional Diffusion Problems

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A large number of observations confirmed the presence of super- and subdiffusive phenomena in the last decades [1]. As a true mathematical model of these, the space-fractional differential equations were proposed using fractional Laplacian [2]. The numerical treatment of these equations is the focus of the talk. First we mention some convergence results for a straightforward approximation, called the matrix transformation method [3]. We discuss then an efficient method to deal with the corresponding linear systems.

Acknowledgments The author is grateful for the support of the project HU-MATHS-IN – Intensification of the activity of the Hungarian Industrial Innovation Mathematical Service Network (EFOP-3.6.2-16-2017-00015).

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On Solvability of Initial-Boundary Value Problem for one model of Viscoelastic Fluid with Fractional Derivatives

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We consider the mathematical models of dynamics of viscoelastic fluid with constitutive relations which contain fractional derivatives. Fractional analogous of Voigt and anti-Zener models are under investigation. We establish the existence and in the planar case uniqueness of weak solutions of the corresponding initial-boundary value problems. Constitutive equations of the models under consideration contain fractional derivatives an are fractional analogous of Voigt and anti-Zener models of viscoelasticity. An approximation of the problem under consideration by a sequence of regularized systems of Navier-Stokes type and the following pass to the limit are used. This is a joint work with Victor Zvyagin.

Acknowledgments This research was supported by the Ministry of Education and Science of the Russian Federation (grant 14.Z50.31.0037).

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Numerical Solution of the Black-Scholes Equation with Distributed Order in Time

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The Black-Scholes (BS) model for pricing stock options was developed by Black F. and Scholes M. [1] and Merton R. [2] in the early 1970's. It is arguably the most important result in finance, and is certainly a rich source of interview in the financial services industry. The BS model provides an approximation of the behaviour of the underlying asset. Although the option price derived by BS model is shown to have a very good agreement with the observed prices, it still has well-known shortcomings such as the failure of capturing the significant movements or jumps over small time steps in a financial market.
In this work we consider the fractional Black-Scholes model with derivative in time given in the distributed sense:

$$\begin{cases} \displaystyle\int_0^1 c(\alpha)\frac{\partial^{\alpha,\lambda}}{\partial t^\alpha}V(x,t)d\alpha + \frac{1}{2}\sigma^2x^2\frac{\partial^2}{\partial x^2}V(x,t) + Rx\frac{\partial}{\partial x}V(x,t) - RV(x,t) = 0, \\ (x,t)\in(0,\infty)\times(0,T) \\ \\ V(0,t)=p(t), \quad V(x,T)=g(x), \quad \lim_{x\to\infty}V(x,t)=q(t) \end{cases} \tag{2}$$

where $V(x,t)$ is the European option price at asset x and at time t, the parameters $T>0$, R and $\sigma\geq 0$ are the maturity time, risk-free rate and volatility function of underlying asset, respectively. The way that functions p, g and q are defined depends on the cases where V is a call or a put option ([2]). The tempered fractional derivative $\dfrac{\partial^{\alpha,\lambda}}{\partial t^\alpha}u(x,t)$ is a modified right Riemann-Liouville tempered fractional derivative of order α, $\alpha\in[0,1]$, and tempered parameter $\lambda>0$ defined as $\dfrac{\partial^{\alpha,\lambda}}{\partial t^\alpha}u(x,t) = \dfrac{e^{-\lambda t}}{\Gamma(1-\alpha)}\dfrac{d}{dt}\displaystyle\int_t^T \frac{e^{-\lambda s}u(x,s)-e^{-\lambda T}u(x,T)}{(s-t)^\alpha}ds.$
In order to approximate the fractional Black-Scholes equation (2), an implicit numerical method is presented and applied to some numerical examples to illustrate the accuracy and effectiveness of the proposed method. We also use the model (2), with several weight functions, $c(\alpha)$, and tempered parameters, to price several European options.

Acknowledgments The author M. Rebelo would like to thank the funding by FCT-Portuguese Foundation for Science and Technology through the project UID/MAT/00297/ 2013. L. Morgado wish to thank FCT through the project UID/Multi/04621/2013.

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MS 02: Qualitative Properties of Ordinary and Partial Differential Equations and their Numerical Solutions

Embedded Error Estimation and Adaptive Step-Size Control for Optimal Explicit Strong Stability Preserving Runge-Kutta Methods

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We construct a family of embedded pairs for optimal strong stability preserving explicit Runge–Kutta methods of order $2 \leq p \leq 4$ to be used for numerical solution of spatially discretized hyperbolic PDEs. In construction, we aims for non-defective methods, large region of absolute stability, and optimal error measurement values. The new pairs offer the ability for strong stability preserving (SSP) methods to be adaptive and take variable step-size based on the local error estimation while maintaining their inheritant nonlinear stability properties. Considering accuracy, efficiency, and stability, the overall effectiveness in term of precision versus work is assessed through several numerical experiments.

Acknowledgment The author is grateful for the support of the project HU-MATHS-IN: Intensification of the activity of the Hungarian Industrial Innovation Mathematical Service Network (EFOP-3.6.2-16-2017-00015).

A Nonlinear Finite Volume Scheme Preserving Maximum Principle

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The maximum principle is one of the key requirements to discretization schemes, and can ensure that there is no spurious oscillations for the numerical solution and preserve physical bounds of problem [1, 2]. For the construction of nonlinear finite volume schemes preserving maximum principle for diffusion equations on distorted meshes, the nonlinear weighted method is a common-used approach. In this talk, we introduce three finite volume schemes preserving maximum principle based on nonlinear weighted methods, in which a conservative flux is constructed by using three kinds of weighted combination of nonconservative flux. We perform an elementary analysis to compare the errors of flux for these weighted methods. Numerical results are presented to demonstrate the accuracy and properties of these schemes [3].

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Qualitative Properties of Linear and Nonlinear Discrete Mesh Operators and their Qualitative Properties

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Some real-life problems of e.g. physics, biology and chemistry are frequently modeled with partial differential equations. These equations are solved with numerical techniques, where in addition to the convergence, we have to ensure some basic characteristic qualitative properties of the original phenomenon. For parabolic problems the main qualitative properties are the non-negativity and non-positivity preservation properties, the different types of maximum-minimum principles and the maximum norm contractivity property. In paper [1], we formulated the above qualitative properties for linear continuous parabolic operators and linear discrete mesh operators, and revealed the relations between them. We formulated sufficient conditions that ensure all of the investigated properties and tested the results on some numerical simulations. In [2], we generalized our previous results for nonlinear continuous parabolic problems, and this generalization for nonlinear discrete mesh operators is done in this presentation. Some parts of this presentation are joint works with István Faragó, János Karátson and Sergey Korotov.

Acknowledgments This research was supported by the Hungarian Scientific Research Fund OTKA, No. 112157.

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On the Stability of Non-Autonomous Systems

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In the first part of this work we present some basic definitions and theorems from the theory of the exponential dichotomy with respect to linear (non-autonomous) systems. After that we are going to study some stability notions of linear differential equations based on the concept of the exponential and ordinary dichotomy. More precisely we are going to see how can we generalize the definition of the asymptotically (Lyapunov-) stability using the exponential dichotomy.

Acknowledgments The author is grateful for the support of the project HU-MATHS-IN – Intensification of the activity of the Hungarian Industrial Innovation Mathematical Service Network (EFOP-3.6.2-16-2017-00015).

A Two Dimensional Model for the Ecological Collapse of Easter Island

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In recent years numerous papers and books discussed the events that led to the demographic collapse on Easter Island taking place in the 16th and 17th century. Most of them visualized a scenario in which the reckless consumption of goods provoked the catastrophic events. However, in the early 2000s Hunt proposed a new theory in which the collapse was caused not only by people, but also the rats brought by the settlers which ate the seeds of the trees.

The theories of Hunt were formalized by Basener et al. ([1]) as a system of differential equations, in which they included the diffusion of the people and the rats on the island. However, we know that because of wind and animal presence, the trees will also have some kind of diffusion. In this way, we expanded their model adding the aforementioned diffusion.

Previously we extended the original Basener model in which the island is thought of as a disc ([2]). This time we construct a system of partial differential equations and examine whether the properties proved in the case of the model of the disc also hold in this continuous, two dimensional model.

Acknowledgments The second and the third authors were supported by the Hungarian Research Fund OTKA under grant no. K-112157 and SNN-125119. The first author was also supported by the ÚNKP-17-3 New National Excellence Program of the Ministry of Human Capacities and by the project HU-MATHS-IN – Intensification of the activity of the Hungarian Industrial Innovation Mathematical Service Network (EFOP-3.6.2-16-2017-00015).

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Quasi-Newton Variable Preconditioning for Nonlinear Elliptic Problems

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Nonlinear elliptic problems arise in various physical and other applications where the model describes a stationary state. The most widespread way to solve the discretized problems is some Newton-like iteration, A general approach to construct quasi-Newton methods can be given via spectral equivalence, which makes these methods a kind of variable preconditioning. The talk first summarizes earlier works where uniformly elliptic problems have been considered. Then extensions are shown to complex-valued problems and to various non-uniformly elliptic models.

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MS 03: Differential Equations in Numerical Modelling: From Theory to Application

Stable and Convergent Fully Discrete Interior–Exterior Coupling for Problems Related to Maxwell's Equations

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Maxwell's equations are considered with transparent boundary conditions, for initial conditions and inhomogeneity having support in a bounded, not necessarily convex three-dimensional domain or in a collection of such domains. We also give some outlook on acoustic and elastic wave equations, and on problems with further models coupled to Maxwell's equations.

The numerical method only involves the interior domain and its boundary. The transparent boundary conditions are imposed via a time-dependent boundary integral operator that is shown to satisfy a coercivity property. The stability of the numerical method relies on this coercivity and on an anti-symmetric structure of the discretized equations that is inherited from a weak first-order formulation of the continuous equations. For Maxwell's equations the method proposed here uses a discontinuous Galerkin method and the leapfrog scheme in the interior and is coupled to boundary elements and convolution quadrature on the boundary. The method is explicit in the interior and implicit on the boundary. Stability and convergence of the spatial semidiscretization are proven, and with a computationally simple stabilization term, this is also shown for the full discretization.

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A Low-Rank Integrator for Semilinear Stiff Matrix Differential Equations

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In this talk we address the problem of solving large-scale matrix differential equations. In particular, we consider semilinear stiff problems. We propose a low-rank integrator based on splitting methods to separate the stiff linear part of the equation from the non-stiff nonlinear one. Then the solutions of the subproblems are approximated by low-rank ones. An efficient exponential integrator based on Leja interpolation is employed for the solution of the linear subproblem. The nonlinearity is handled by means of the so-called projector-splitting integrator which is an integrator to efficiently compute time-dependent low-rank approximations. We provide a convergence analysis of the presented scheme and show some numerical results. In particular, we discuss the simulation of the weather phenomenon El Niño. We mainly refer to [1].

This is joint work with A. Ostermann and L.-M. Pfurtscheller (University of Innsbruck), H. Mena (Yachay Tech, Ecuador), and H. Walach (University of Tübingen, Germany).

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Flood Prevention with Mathematics

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One of the serious impacts of climate change is the increasing number of severe floodings, therefore, flood prevention is becoming increasingly important. After an earthquake or just a heavy rain a flood appears on the surface of the sea, the lake, or the river's water. Its movement can be predicted by the solution of partial differential equations coming from the theory of hydrodynamics. Such events can be described by the linearized shallow water equations being a reasonable simplification. Flood prevention can be considered as adjusting water height to normal. Mathematically, this means an optimal control problem. The change in the water height is then described by the corresponding linear quadratic regulator problem.

In the talk we present our results concerning the efficient way to solve the linear quadratic regulator problem related to the linearized shallow water equations by using an operator splitting procedure and an exponential integrator. We prove the methods' convergence [1], and show several numerical experiments illustrating our results [2]. Since the convergence proof requires the operator, appearing in the abstract form of the linearized shallow water equations, to be a generator of a strongly continuous operator semigroup, we briefly outline the relevant proof [3].

Acknowledgments The author is grateful for the support of the National Research, Development and Innovation Office (grant MAT-PD-117121).

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A Local Time Stepping Method for District Heating Networks

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District heating is an efficient and sustainable alternative to conventional heating systems. For the optimal control of these networks a fast and accurate forward simulation is important.

In this talk we want to present a new solver for simulations of district heating networks. The numerical method applies the local time stepping introduced in [1] to networks of linear advection equations. Numerical diffusion as well as the computational effort on each edge is reduced significantly. In combination with the high order coupling approach of [2] an accurate and very efficient scheme is developed. In several numerical test cases the advantages for simulations of district heating networks are shown.

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A Split Step Fourier/Discontinuous Galerkin Scheme for the Kadomtsev-Petviashvili Equation

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In this talk we introduce an efficient and explicit method for the Kadomtsev–Petviashvili equation. In particular, the method is not encumbered by a CFL step size restriction. This is accomplished by splitting the linear part from the nonlinear part. The latter is then treated by a semi-Lagrangian discontinuous Galerkin approach of arbitrary order. This is, to our knowledge, the first application of a semi-Lagrangian scheme to a problem where the advection speed depends on the solution itself.

We demonstrate the efficiency and accuracy of the numerical method by providing a range of numerical simulations. In particular, we find that our approach can outperform the numerical methods considered in the literature by up to a factor of five. Although we focus on the Kadomtsev–Petviashvili equation in this talk, the proposed numerical scheme can be extended to a range of related models as well.

This talk is based on [1, 2].

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Comparative Study of Heuristic Algorithms for Electrical Impedance Tomography

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Electrical Impedance Tomography (EIT) is a non-invasive imaging technique in which the conductivity distribution within a body is reconstructed given measurements of electrical current and voltage around its boundary. Traditional deterministic solvers for the EIT problem were found to perform poorly under realistic conditions and are heavily dependent on the initial guess and the gradient of the cost functional. Recent studies have shown promising results in reconstructing EIT images using heuristic algorithms, demonstrating their superior performance over traditional solvers in terms of reconstruction accuracy. This work presents a comparative performance study of five heuristic algorithms - simulated annealing algorithm, differential evolution algorithm, genetic algorithm (GA), novel bat algorithm, and firefly algorithm - for the EIT image reconstruction problem. Series of numerical tests were carried out to investigate and compare the performance of these algorithms, for the cases where the inclusion/s in a unit square domain is/are (1) a rotated ellipse, (2) an irregular shape, and (3) two irregular shapes. In addition, a two-step approach is adopted by hybridizing the best heuristic algorithm based on chosen performance measures with a modified interior-point method.

Acknowledgments The authors are grateful for the financial support by the Department of Science and Technology (DOST) Science Education Institute (SEI) under the Accelerated Science and Technology Human Resource Development Program (ASTHRDP) National Science Consortium (NSC) Student Research Support Dissemanation Grant and the Natural Sciences Research Institute (NSRI) of the University of the Philippines Diliman under Project Code: MAT-16-1-01.

Numerical Analysis of a Monotone Ddfv Scheme for the Richards Equation

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The Richards equation occurs in modeling unsaturated flows in porous media [1, 2]. It is a degenerate nonlinear parabolic equation. In order to approximate it in two dimensional in space, we design a new discrete duality finite volume (DDFV) scheme which has been introduced in [3] and analyzed later on in [4, 5]. The basic idea rests upon different approximations of the fluxes on the same interface of the control volume. Precisely, the approximate flux is split into two terms corresponding to the normal and the tangential components. Then the first term is discretized using a centered scheme whereas the second one is approximated in a non evident way with the help of an upwind scheme.

The strength of this approach consists in preserving the physical bound of the computed solution on almost general meshes and for anisotropic permeability tensors. This allow us also to derive energy estimates on the discrete gradient of the Kirchoff transform functions which is a fundamental result to carry out the analysis of the numerical scheme. Next, we prove that the scheme possesses an approximate solution, which converges toward the weak solution of the continuous problem as the steps of the time-space discretisation tend to zero. Some numerical tests are ultimately provided so that one can ensure the accuracy and the stability of our method.

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MS 04: New Trends in Education

Virtual Academic Mobility in the context of the Master's Program "Computational Mechanics and Information Technologies" in the Southern Federal University

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Southern Federal University (SfedU) is a leader university in South of Russia and is in the top list of the Russian universities. SFedU combines studies with fundamental and applied science, as well as cutting-edge technologies and innovative approaches. The University's position in the national university rankings provides persuasive evidence to its achievements, a positive image and a passion for excellence [1]. Since 2015 SFedU was included in the QS World University Ranking [2].

School of Mathematics, Mechanics and Computer Science is one of the oldest, biggest and powerful institution of SFedU with great achievements in mathematics, mechanics and their applications. School involves more than 1000 students in Bachelor, Master and Doctoral programmes. Approximately 100 academics and 30 staff provide education and research in different fields of applied mathematics, mechanics, information technologies and computer science. There are many good examples of successful interaction with foreign universities in the "portfolio" of the School.

In the past the School's interactions mostly were within the Russia, but now they become more international and open-minded. Now we are in preparation to launch new Master Programme "Computational Mechanics and Informational Technologies" which will be taught in English.

The presentation provides the concept of this Master Programme and ways of their implementation. In this master's program an important place is given to international academic mobility and interaction with foreign partner universities. Using the Internet gives new opportunities for "virtual mobility", remote interaction and distance learning. The presentation discusses some problems in the organization of virtual, remote and distance education and ideas how to solve these problems.

The other aim of the presentation is to provide the information about the Southern Federal University and the School of Mathematics, Mechanics and Computer Sciences and find new partners among foreign universities and academics. Also presentation contains a number of examples that demonstrates our achievements in education and solving various problems in mechanics, mathematical modelling and computer science.

Acknowledgments The Master Programme "Computational Mechanics and Informational Technologies" is supported by a grant from the Vladimir Potanin Charity Fund (project GPK-96/17). The authors are grateful for this financial support.

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The ECMI Modelling Weeks

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One of the most successful ECMI events, connected to education, is the traditional ECMI Modelling Week that takes place every summer. International teams of students (mainly from the MSc programs of the ECMI Centers) work intensively for a week in order to solve challenging applied problems under the guidance of instructors from all over Europe. Bulgaria had the great opportunity to host the event in Sofia in July 2016. It gathered together about 60 students and 10 instructors from the ECMI Centers. A very positive result was the fact that a further collaboration was established between one of the instructors and some of the students he guided during the week.

In the present talk, the Bulgarian experience of organizing such an event will be shared. Then, we shall comment on the benefits for the students by trying to find out what role the Modelling Week played for their future careers. The latter will be done on the basis of several students' and instructors' testimonials. Also, some ideas will be presented and a discussion will be encouraged for the possible ways that the collaborations, established during the event, can be further strengthened and used.

Modelling Workshops from a Student's Perspective

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During my Bachelor and Master studies I have attended to the ECMI Modelling Week 2014 at Universität Paderborn as well as the first year's MODCLIM (Modeling Clinic for Industrial Mathematics) project 2015 at Universidad de las Palmas de Gran Canaria (ULPGC) and Lappeenrante University of Technology (LUT). Both events deal with mathematical modelling projects and are addressed to students. The ECMI Modelling Week is an annual one-week workshop, where small groups of students from all over Europe work together on a problem. MODCLIM is a two year Erasmus+ project for PhD and advanced undergraduate students consisting of a training course and problem solving workshop dealing with projects from industry.

The aim of this talk is to describe these experiences from the point of view of a student participating there and explaining the advantages and personal benefits of those type of projects based on my own experience.

Designing Three Math MOOCs for Stem Students

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In the past couple of years,Técnico Lisboa of Universidade de Lisboa (tecnico.ulisboa.pt) has been aiming to position itself in the latest developments of Massive Open Online Courses (MOOC) with a definition of a strategic plan. This strategy takes into account both the Portuguese higher education context in the areas known as Science, Technology, Engineering, Mathematics (STEM) and, on the other side, the education in STEM elsewhere in the world. The first online courses were launched by the end of October 2016 in a proprietary platform MOOC Técnico (mooc.tecnico.ulisboa.pt) based on Open edX. Over a period of one year and few months, eight online courses were produced and run for the first time, several of them even resulted in successfully reruns, with seven more courses under production and scheduled for launching during 2018. Around 4000 participants are presently enrolled in the online courses.

Among these courses, there are already three Math MOOCs: Markov Matrices (mmX) and Eigenvalues (vapX) aimed to undergraduates, and Optimal Stopping Problems (ospX) aimed to graduate students in general, and to ECMI enrollees in particular. The mmX course, the first MOOC Técnico course, is an introductory MOOC to stochastic matrices and to PageRank matrix model, and underwent already three successful reruns. It goes now in a self-paced mode and was the first MOOC to use an innovative assessment system of quizzes. The vapX course, launched in November 2017, was used within a flipped-class experiment with on-campus students enrolled in a Linear Algebra standard course that achieved very good learning results. Finally, the ospX course is one of the MOOCs which is under production and soon to be launched. It aims providing students the mathematical tools to solve optimal stopping problems, with special focus on finance and economics applications.

In the New Trends in Education (ECMI) mini-symposium we, as authors of the three Math online courses, share our testimony about the observed practices, our own, and the team members (including the technical multimedia team) involved in designing and producing each mentioned online course (mmX, vapX and ospX). Preliminary conclusions with corresponding indications for future work are underlined, in a perspective of research-action towards the improvement of guidelines for MOOC courses and video contents. We will then attempt to answer the following questions: a) which factors were key factors for the curricular organisation of the given MOOC? b) which of the following moments had our preferencial care in the MOOC: videos or texts, learning online objects, interaction moments, assessment? c) which of the following items have we spent more time on during the pre-production of our MOOC: video storyboards or/and texts, preparing slides, planning graphics or/and other multimedia contents, preparing peer review topics, preparing discussion topics, preparing questions for quizzes? d) How did we feel about the collaborative work of designing and producing a MOOC within a pedagogical-technical multimedia team?

Challenges of Teaching Mathematics in XXI Century

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Copybook, textbook, pencil, ruler – this basic set of student tools combined with the teacher writing with chalk on the blackboard do not always go along the most exciting mathematics class experience. The ways of teaching of mathematics have been changing rapidly at different education levels due to a number of factors, such as the spread of new pedagogical approaches, development of teaching technology and the overall digitalization in the world. This is very prominent in university education where more and more emphasis is put towards place-independent student-centered studying.

Nowadays the students are exposed to a much bigger variety of learning and assessment tools, many digital-based, which forces them to revise the ways in which they engage in learning [1]. Especially at the university level, a huge emphasis is put on development of students' universal soft skills along learning the actual substance of any course. The teaching tools and methods have, in turn, a huge influence on student satisfaction and overall performance in the class.

Technology can support mathematics teaching in many ways, for instance, in preparation of various presentations helping visualization of new concepts, solving problems or verification of solution correctness, possibility of preparing online teaching materials, creating games with learning purpose, among many others [2].

However, many questions remain to be answered along the changes happening. Are the new pedagogical methods and technological tools easily adopted in the classrooms and is the success of the use dependent on the teacher generation? How much do the modern methods actually enhance the teaching/learning process and how are they in general perceived by the teachers and students? Do the students perform better when exposed to advanced teaching tools or is the classical blackboard and pen-and-paper approach the most efficient approach after all? This presentation will discuss these matters and will give subjective answers to them.

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MS 05: Mathematical Modeling of Vector-borne Disease Transmission

Designing Simple Epidemic Models for Better Data Assimilation

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We utilize a host–vector model with a constant total human population to model dengue epidemic data from Jakarta (time horizon January 2008 week 1 – February 2018 week 4). The unobservable parameters in the model determine which trend the model solution can be adjusted to follow. More specifically as the virtue of a typical inverse problem, certain designs over the unobservable parameters can be initiated towards reasonable data assimilations. Owing to extracting the leading Fourier frequencies of the data, we design the infection rate as in two forms: a piecewise constant function to let the model solution delineate a single outbreak within every year-wide data and a linear combination of sinusoidal functions to catch multiple outbreaks from data with a wider horizon. To compensate model–driven bias in the data assimilation results, we investigate the relationship between the infection rate and some external entities contributing to the rise of the epidemics, which also results in the correction in the prediction. Due to granted free access to hospitals at the end of 2015, a more intense flow of dengue patients were directed to hospitals, rendering a correction to the number of cases as of the moment backwards. We then imported the idea of generating good forecast to calculate such correction factor.

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An Agent Based Modeling of Spatially Inhomogeneous Host-Vector Disease Transmission

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In this article we consider a microscopic model for host-vector disease transmission based on configuration space analysis. We model transmission with birth-death in vector and mobility in host. Using Vlasov scaling we obtain the corresponding mesoscopic (kinetic) equations, describing the density of susceptible and infected compartment in space. The resulting system of equations can be seen as a generalization to a spatial SISUV model. Furthermore, we develop the estimation of basic reproduction number from the kinetic equations. In this approach we may obtain the local and global basic reproduction number of infectious disease.

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Integrating Daily Dengue Incidence, Rainfall and Relative Humidity Data for Early Detection of Dengue Outbreak

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Dengue fever has been identified by WHO as the most rapidly spreading mosquito-borne disease in the world with an estimated fifty million dengue infections occurring annually. Although intervention and prevention programs have been conducted continuously, the spread of the dengue virus is still increasing in many regions, especially in tropical and sub-tropical countries. One of the main source of the difficulty in predicting the dengue cases is due to the unavailability of mosquito data which is highly affected by the changing of rainfall, humidity and temperature. Basic reproductive ratio is commonly used as the main indicator for identifying and predicting the level of dengue endemicity, which is constructed under uniform conditions. With the changing of weather condition, the standard basic reproductive ratio is no longer valid for measurement. We construct here a time dependent basic reproductive ratio based on a reduced SIR dengue dynamic and estimate that ratio based on the dengue daily incidence, rainfall and humidity data in Jakarta. The results are expected for early detection of dengue outbreak.

Acknowledgments The author is grateful for the support of the RistekDikti-ITB Research Grant.

Analysis of Vector-Bias and Blood Resource Dependence in Malaria Disease Model with Mosquito Repellent

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Vector-bias effect on mosquito-borne disease transmission occur when mosquito is more attracted to bite infected human [1, 2, 3]. The aim of this talk is to investigate how blood resource dependence and vector-bias effect affects the changes in the dynamic of malaria and how mosquito repellent should be implemented to control the malaria transmission. Mathematical model analysis about the existence and local stability of equilibria will be discuss related to the basic reproduction number. Our results showed that the mosquito repellent use can work to eliminate the disease only if the effectiveness of the mosquito-repellent is high enough to satisfy some condition which depend on basic reproduction number and the mosquito-intrinsic net reproductive rate.

Acknowledgments This research was financially supported by the Indonesia Ministry of Research and Higher Education (Kemenristek DIKTI), with PUPT research grant scheme 2018.

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Comparison of Host Immune Responses on the Behavior of Dengue Viral Dynamics

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Dengue virus is an arthropod-borne virus that has become a major global public health challenge in the tropical and subtropical countries throughout the world. It was recently estimated that around 390 million dengue infections occur annually [1]. Despite this, the dengue pathogenesis and the immune response during dengue infection is not well understood. Currently there are no vaccines or anti-viral drugs available against dengue [2]. Vaccine development has been hampered by lack of understanding of the complex nature of the host immune response. Extensive research has been done to model the transmission dynamics of dengue. However only a limited number of models exists for within-host dengue pathogenesis due to the complex interactions between virus and immune response. Mathematical modeling of interaction between virus and immune response is a powerful tool for understanding the host immune response during infection and for the rational development of antivirals or vaccines. In this paper, we developed a conceptual mathematical model combining all aspects of the immune system where immunity is provided by innate immunity, antibody mediated immune response and cell mediated immune response. Simulations were done by modifying the model to observe the impact of different immune responses on viral dynamics. Three different behaviors were identified. In the first case it was assumed that immunity is provided only by antibody mediated immune response. In this case, only one virus titer peak was observed and a significant delay in production of antibodies was noted. Also it was observed that the virus count goes to negligible levels within 7-14 days after the onset of symptoms. In the second case, it was assumed that immunity is provided by innate immune response and antibody mediated immune response. In this case, two virus titer peaks was observed. In the third case it was assumed that immunity is provided by innate immunity and cell mediated immunity and only one virus peak was observed. A comparison was done between the full model and each individual model to understand the virus dynamics produced by different immune responses.

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Compartmental Spatial Multi-Patch Deterministic and Stochastic Models for Dengue

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Dengue is a vector-borne viral disease increasing dramatically over the past years due to improvement in human mobility. The movement of host individuals between and within the patches are captured via a residence-time matrix. A system of ordinary differential equations modeling the spatial spread of disease among the multiple patches is used to create a system of stochastic differential equations (SDE). For this model the basic reproduction number is derived, giving a choice for parameters in the endemic case. Numerical solutions of the system of SDE are compared with the deterministic solutions.

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Modelling Dengue Fever with the SIR Model

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Severe dengue outbreaks and their consequences point out the need for prognosis and control methods which can be derived by epidemiological mathematical models. In this talk we develop a model to describe observed data on hospitalized dengue cases in Colombo (Sri Lanka) and Jakarta (Indonesia). Usually, the disease is epidemiologically modelled with the SIRUV model consisting of the susceptible S, infected I and recovered humans R and the uninfected U and infected V female mosquitos. Because we do not have any information about the mosquito population we reduce the model to a SIR model which depends on a time-dependent transmission rate $\beta(t)$. In order to fit the parameters of the model to the received data sets we implement an objective function

$$J(u) = \int_0^T \big(I(t) - data(t)\big)^2 dt + \frac{\|u\|^2}{N^2}$$

which shall be minimized. This optimization problem depends on u – which includes the parameters that shall be fitted – and on the ODEs of the SIR model. To solve this, optimal control theory constructed on Pontryagin's maximum (minimum) principle is applied in order to reach the solution with numerical optimization methods. The results serve as a basis for different simulations concerning the number of dengue fever cases.

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MS 06: ECMI Special Interest Group: Mathematical Modelling in Biomedical Applications

Modelling Drug Release from Polymer-Free Stents with Microporous Surfaces and Drug-Filled Stents

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Polymer-free drug-eluting stents (DESs) are an innovative new treatment for cardiovascular disease which is the leading cause of death globally. They have the potential to overcome problems associated with the traditional polymer-coated DESs (e.g. late stent thrombosis). However, the absence of a rate-controlling polymer layer makes optimisation of the drug release profile a particular challenge. The use of microporous stent surfaces to modulate the drug release rate is an approach that has recently shown particularly promising clinical results. A mathematical model has been developed to describe drug release from stents with microporous surfaces. The model predicts a two-stage release profile, with a relatively rapid initial release of most of the drug, followed by a slower release of the remaining drug. In the model, the slow release phase is accounted for by an adsorption/desorption mechanism close to the stent surface. The theoretical predictions are compared with experimental data and good agreement is found.

The model of drug elution from a drug-filled stent is also developed. The drug is stored in the inner layer of a tri-layer wire which acts as a reservoir releasing the drug through laser-drilled holes on the outer surface of the stent struts. The general model is simplified using the assumption of low drug solubility and two special cases where the dissolution occurs in a uniform downward direction and in a spherical outward direction are considered. The main advantage of the simplified models is the ability to achieve analytical solutions. These solutions allow for calculating the drug release profile rapidly and for identifying the dependence of the various parameters of the system.

The valuable insights provided by these models will serve as a useful guide for designing the enhanced polymer-free stents of the future.

Acknowledgments The research project supported by the Science Foundation Ireland (SFI) Investigator Award (grant number 12/IA/1683), the New Foundations Award 2013 and 2014 from Irish Research Council, the Royal Society (grant reference IE131240), and EPSRC (grant number EP/J007242/1, EP/J007579/1 and EP/F50036X/1).

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Modelling Biology After Implantation of a Drug Eluting Stent

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A standard treatment for atherosclerosis is percutaneous balloon angioplasty in which an occluded artery is reopened by inflating a balloon inside it. To prevent the artery narrowing again (restenosis) a drug eluting stent is deployed within the artery. The stent mechanically holds the artery open, while also releasing drugs which inhibit cell proliferation which can lead to restenosis. A long time goal of the research community has been to develop mathematical models that could be used to optimise stent design. These models would be able to predict mechanical stresses due to blood flow, especially wall shear stress [1], diffusion of the drug through the artery wall [2] and the cell biological aspects of restenosis. Here we present preliminary results of adapting cell biology models developed for tumour growth to model the uncontrolled cellular growth leading to restenosis [3].

Acknowledgements We gratefully acknowledge the support of the Mathemat- ics Applications Consortium for Science and Industry (www.macsi.ul.ie) funded by the Science Foundation Ireland (SFI) Investigator Award 12/IA/1683. Dr Vo also thanks the New Foundations Award 2013 and 2014 from Irish Research Council.

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Modeling the Effect of Flow on the ATP/ADP Concentration at the Endothelial Cell Surface

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The nucleotides ATP and ADP regulate many aspects of endothelial cell (EC) biology, including intracellular calcium concentrations, focal adhesion activation, cytoskeletal organization, and cellular motility. In vivo, ECs are constantly under flow, and the concentration of ATP/ADP on the EC surface is determined by the combined effects of nucleotide convective and diffusive transport as well as hydrolysis by ectonucleotidases on the EC surface. In addition, experiments have demonstrated that flow induces ATP release from the cells. Previously computational models have incorporated the above effects and thus described concentration at the EC surface. However, it remains unclear what physical processes are responsible for nucleotide regulation. While some EC responses to flow have been shown to be directly driven by shear stress, others appear to also involve a non-negligible contribution of transport. In the present work, we develop a mathematical model and perform numerical simulations to investigate the relative contributions of shear stress and transport to nucleotide concentration at the EC surface, with the effect of cell density. Because in vitro experiments are performed by using confluent cells in some cases and subconfluent cells in other cases, we also investigate the effect of cell density on the results. The outcomes of the simulations demonstrate a complex interplay between shear stress and transport such that transport has a significant contribution at certain shear stress values but not at others. The effect of transport on nucleotide concentration increases with cell density. The present findings enhance our understanding of the mechanisms that govern the regulation of such molecules at the EC surface under flow. The implications of these findings for downstream responses such as cellular motility merit future investigation.

Electrical Conduction in Media with Microstructures

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Often problems of electrical conduction arise in media containing a periodic array of inclusions; for example in biological tissues the inclusions are the cell membranes, which are insulating, and the matrix, which is conductive, is given by the extra- and intra-cellular spaces. A simplified geometry of this setting is given therefore by insulating spherical shells surrounded by conductive phases.

We give here a more explicit statement to our problem. Let u be the electric potential; then in the conductive phases we have

$$\lambda \nabla^2 u = 0\,,$$

where $\lambda > 0$ may actually depend on the position and ∇^2 is the laplacian.

In the insulating or dielectric part we assume

$$\alpha \nabla^2 \frac{\partial u}{\partial t} = 0\,,$$

where $\alpha > 0$ and t is the time variable.

We prescribe continuity of the current at interfaces

$$\lambda \nabla u \cdot \nu = \alpha \nabla \frac{\partial u}{\partial t} \cdot \nu$$

on the boundaries between insulating and conductive phases, where ν is the normal unit vector to the interface.

This problem may be *concentrated*, that is the dielectric shells are approximated by surfaces. Besides this, our interest here is in the *homogenization limit* of this model, when we let the period of the array of dielectric inclusions become vanishingly small. We'll see that the topology of inclusions plays an important role.

The homogenization limit yields in fact a non-standard partial differential problem with memory.

Mathematically Modeling Drug Release from Solid Dispersions

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A solid dispersion refers to a dosage form where an active ingredient (a drug) is mixed with at least one inert solid component. The purpose of the inert component is usually to improve the bioavailability of the drug. In particular, the inert component is frequently chosen to improve the dissolution rate of a drug that is poorly soluble in water. The construction of reliable mathematical models that accurately describe the dissolution of solid dispersions would clearly assist with their rational design. However, the development of such models is challenging since a dissolving solid dispersion usually consitutes a non-ideal mixture, and the selection of appropriate forms for the activity coefficients that describe the interaction between the drug, the inert matrix, and the dissolution medium is delicate. In this talk, we model the stability of a solid dispersion in storage. The dispersion consists of a drug in an inert polymer, and Flory-Huggins theory is used to derive an expression for the activity coefficient. The mathematical model ultimately consists of a nonlinear partial differential equation for the drug, and we analyze this equation numerically and analytically to identify parameter regimes that lead to the undesirable phenomenon of phase separation.

Modelling Protein Adsorption and Optimisation of Novel Immunodiagnostic Devices

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Current immunodiagnostic devices often rely on the physical adsorption of detection antibodies on solid substrates for binding analytical targets such as pathogenic organisms, hormones or protein biomarkers for cardiovascular disease or cancer. However, it is widely acknowledged that the binding efficiency of immobilized antibodies is severely compromised due to improper orientation of the particles and conformational changes upon contact with the substrate.

A mathematical and computational modelling framework, based on the theory known as Random Sequential Adsorption, as well as novel techniques, has been proposed in [1], [2] in order to describe the distribution and orientation of adsorbed particles and quantify their activity and assay response. This talk will explore the development and applicability of generalized mathematical models to ongoing experimental work for monitoring analytes such as PSA (prostate-specific antigen), [3], through new strategies such as immobilization on magnetic nanoparticles, creation of single-chain antibody fragments, molecular tethers for allowing rotational flexibility, etc.

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MS 07: Mathematical Modelling in the Silicon Industry

Approaching Solidification Fronts in the Extended Stefan Problem for Binary Alloys in Finite Domains

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The manner in which an alloy solidifies has an impact on its microstructure, and thus on the quality of the final product. In order to gain an understanding of this process, we consider a model for the solidification of a binary alloy which accounts for constitutional supercooling. Although a similarity solution exists when the problem domain is semi-infinite, in practice solidification problems related to many real-world applications are posed on finite domains. We consider the solidification of a binary alloy on a symmetric one-dimensional planar domain, finding that two identical solidification fronts start from each boundary and move inward toward one another. Then, we perform an asymptotic analysis to better understand the solidification front dynamics. The two fronts are initially far from one another and move in a self-similar manner toward the interior of the domain for small time. However, when the two fronts are sufficiently close, there is a build-up of impurities in the liquid phase between the fronts, which increases the supercooling and thereby slows the fronts. Eventually, the system evolves to its minimum temperature, with the liquid phase following in thermodynamic equilibrium. The asymptotic solutions show excellent agreement with numerical simulations of the full problem, as well as with experimental data involving the solidification of silicon in a cast. Our analysis highlights the important role of supercooling in the solidification of binary alloys.

Acknowledgments This presentation is on work supported by the EPSRC Centre For Doctoral Training in Industrially Focused Mathematical Modelling (EP/L015803/1) in collaboration with Elkem AS.

Heat Transfer and Chemical Reactions in a Silicon Furnace

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Silicon is produced from quartz rock in electrode-heated furnaces by using carbon as a reduction agent. We have developed a model of coupled PDEs which captures the evolution of chemical concentrations, temperature, and gas partial pressures and flow, within a pilot furnace [1]. This model has been analysed in two ways. Firstly by numerical simulations, and secondly by asymptotic analysis. The numerical simulations compare well with experiments, and give insight into how the silicon yield can be increased by using more reactive carbon. The asymptotic analysis highlights the strong coupling between the chemistry and temperature and includes diffusion, an endothermic reaction, and the external heating input to the system [2]. We comment on how the findings may be relevant for the operation of silicon furnaces.

Acknowledgments This talk is based on work supported by the EPSRC Centre for Doctoral Training in Industrially Focused Mathematical Modelling (EP/L015803/1) in collaboration with Elkem.

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Lumped Modelling of Three-phase AC Smelting Furnaces

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We study the use of simple circuit models of general three-phase AC smelting furnaces. The focus is on submerged arc furnaces, for instance used in the production of ferromanganese or ferrosilicon. The general framework can, however, be applied to other three-phase furnaces. A lumped model is solved fast, thus it allows us to investigate the effect of changing parameters in real time. Lumped models may be related to the measurements that are made on real furnaces, and may be used in process control [1, 2]. In this work, we define an equivalent circuit model for the current flow in a three-phase furnace. We consider both the transformers and exterior connections, as well as the electrodes and furnace interior, as lumped elements. We specify the geometry and resistances for each element. From the defined geometry we calculate the inductances within the furnace, which gives us the impedance of each element. We relate the lumped model to a distributed 3D model, which is solved numerically using Comsol Multiphysics. The relation between a circuit model and a 3D distributed model is not unique. Any 3D axially symmetric current will, for instance, produce the same magnetic field outside the conductor, as a line element with the total current flowing along the symmetry axis [3]. Thus, a circuit model may produce accurate estimates for the magnetic fields outside a conductor. However, it will not be able to reproduce the field within. As a consequence, an important challenge for the circuit model, is to accurately describe the field distribution in the furnace interior.

Acknowledgments This publication is part of the research project Electrical Conditions and their Process Interactions in High Temperature Metallurgical Reactors (ElMet). ElMet is a collaboration between Teknova, University of Santiago de Compostela, University of Oxford, Norwegian University of Science and Technology, and the companies Elkem and Eramet. It is financially supported by the Research Council of Norway and the industrial partners.

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Homogenisation Applied to Electrical Calcination of Carbon Materials

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Calcination describes the heat treatment of anthracite particles in a furnace to produce a partially-graphitised material which is suitable for use in electrodes and for other metallurgical applications. Electric current is passed through a bed of anthracite particles, here referred to as a coke bed, causing Ohmic heating and high temperatures which result in the chemical and structural transformation of the material. To explain behaviour in these furnaces, one must understand how electric current and thermal energy propagate through the granular material within it. This is a complex process due to the irregular and inhomogeneous shapes of the particles, with a particular dependence on the nature of the contacts between particles. The size of such contacts are microscopic in comparison to the scale of the furnace, but their impact on the electrical and thermal conductivity is critical. Therefore, understanding the process on a microscopic level is imperative to understanding the macroscopic behaviour of the furnace.

Through experimental exploration and scaling arguments we have deduced that the electrical resistance at the contacts between particles contributes substantially to the bulk resistivity of the coke bed. Similarly, a sound understanding of thermal radiation between particles is imperative to fully explain the temperature distribution of the material. Understanding the behaviour of such mechanisms on the scale of a single particle is often dealt with through the use of computational models such as DEM (Discrete Element Methods). However, because of the great discrepancy between the length scale of the particles and the length scale of the furnace, we can exploit asymptotic homogenisation theory to simplify the problem. We consider behaviour on the particle length scale (the microscopic scale), and use this to define a homogenised model on the furnace length scale (the macroscopic scale). This produces an effective-medium problem which captures the important features of the problem whilst minimising the complexity.

In this talk, we will present some results relating to the electrical and thermal conduction through granular material which define effective quantities for the conductivities by considering a microscopic representative volume within the material. The effective quantities are then used as parameters in the homogenised macroscopic model to describe calcination of anthracite.

Acknowledgments This publication is based on work supported by the EPSRC Centre for Doctoral Training in Industrially Focused Mathematical Modelling (EP/L015803/1) in collaboration with Teknova and Elkem. This work is part of the research project Electrical Conditions and their Process Interactions in High Temperature Metallurgical Reactors (ElMet), with financial support from the Research Council of Norway and the companies Alcoa, Elkem and Eramet Norway.

MS 08: Mathematics as a Key Factor to Master the Challenges of the Energy Transition

Towards an Input-Aware System-Theoretic Model Order Reduction Approach for Nonlinear Systems

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We propose a new Galerkin-projection based interpolatory model order reduction approach for quadratic-bilinear dynamical systems. In contrast to the approach of multi-moment matching [2] using a series of multivariate frequency representations, we construct, for given inputs, a series of univariate frequency representations and aim for approximate moment matching of the first terms in this representation.

As has been discussed in [3], for quadratic-bilinear systems with certain fixed inputs univariate associated frequency representations can be constructed using the associated transform.We use this idea, but combine it with the notion of a system to be driven by a signal generator [1] to handle far more general scenarios. Herefore, the inputs of interest are represented by a user-defined quadratic dynamical system, the signal generator, and then interconnected to the dynamical system we started with in a cascade. The interconnected system is then a quadratic dynamical system with an extended state consisting of the original state plus the signal generator. For this extended system associated frequency representations can be constructed similarly as in [3].

Convenient formulations of the associated functions, as well as their moments are given. They involve expedient tensor structures and Lyapunov-type equations. We use these representations to construct reduced models achieving approximate moment matching in terms of the associated functions. Numerical examples for our approach will be presented.

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Mathematical Formulation of Stochastic Fluctuations in Gas Networks

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Low cost of natural gas has driven an expansion of gas-fired power plants. Their ability to ramp quickly may be used to balance fluctuations due to renewable energy, which in turn leads to time-varying gas consumption and fluctuations in the gas network. Since gas system operators assume nearly constant gas consumption, there is need to assess the risk of these stochastic fluctuations, which occur on shorter time scale than the planning horizon. We present a mathematical formulation for these stochastic fluctuations being a generalization of isothermal Euler equations. Furthermore, we discuss numerically control policies to damp fluctuations in the network.

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Price-based Predictive Control of Residential Energy Systems using Energy Storage and Controllable Loads

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The rapid uptake of renewable energy sources yields many challenges for electricity distribution networks, see, e.g. [5]. In this paper, we focus on the difficulty to deal with fluctuations from a grid operator's point of view. The grid operator, which can be seen as a central entity, employs time-of-day-tariffs to influence the supply and demand of locally distributed Residential Energy Systems (RESs). Each RES may have a locally installed energy storage device, e.g. a battery, and/or controllable loads – similar to the setting considered in [2]. Hence, the grid operator wants to exploit the *flexibilities* of each RES to mitigate effects resulting from high fluctuations of the aggregated energy demand. To this end, a distributed dual ascent algorithm was developed in [1] to distributedly coordinate the charging and discharging behaviour of the RESs – however, without taking controllable loads into account. Our goal is to extend this approach to the setting including controllable loads. For this purpose, we conduct a case study based on the data from customers in an Australian electricity distribution network on generation, load, and controllable load [3]. Moreover, we numerically investigate the usuage of surrogate models [4] in order to facilitate real-time applicability of our algorithm.

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Index-aware MOR for Gas Transport Networks with many supply inputs

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We consider gas flow through a gas transportation network with more than one supply node and desired demand nodes. The gas network can be modeled by the isothermal Euler equations [2] and, spatial discretization of these equations leads to nonlinear differential-algebraic Equations (DAEs) of the form

$$\mathbf{E}\mathbf{x}' = \mathbf{H}\mathbf{x} + \mathbf{f}(\mathbf{x}) + \mathbf{B}\mathbf{u}, \quad \mathbf{E}\mathbf{x}(0) = \mathbf{E}\mathbf{x}_0, \quad \mathbf{y} = \mathbf{C}\mathbf{x} + \mathbf{h}(\mathbf{x}), \tag{3}$$

where $\mathbf{E} \in \mathbb{R}^{n\times n}$ is singular. $\mathbf{H} \in \mathbb{R}^{n\times n}$, $\mathbf{B} \in \mathbb{R}^{n\times m}$, $\mathbf{C}, \mathbf{h}(\mathbf{x}) \in \mathbb{R}^{\ell\times n}$, $\mathbf{f}(\mathbf{x}) \in \mathbb{R}^n$, is strongly nonlinear and the state vector $\mathbf{x} = \left(\mathbf{x}_q^T, \mathbf{x}_p^T\right)^T \in \mathbb{R}^n$, includes the gas flux $\mathbf{x}_q \in \mathbb{R}^{n_1}$, and the gas density $\mathbf{x}_p \in \mathbb{R}^{n_2}$ within the pipe network. The input function $\mathbf{u} = \left(\mathbf{u}_p^T, \mathbf{u}_q^T\right)^T \in \mathbb{R}^m$, includes $\mathbf{u}_p \in \mathbb{R}^{m_s}$, $m_s > 1$ the supply pressure, and demand mass flow $\mathbf{u}_q \in \mathbb{R}^{m_d}$, respectively. The desired output vector $\mathbf{y} = \left(\mathbf{y_p^T}, \mathbf{y_q^T}\right)^{\mathbf{T}} \in \mathbb{R}^\ell$, includes the supply mass flow $\mathbf{y}_p$ and the demand pressure $\mathbf{y}_q$. We are interested in a fast and stable prediction of the dynamics of natural gas transport in the pipe networks, and therefore the application of model-order reduction (MOR) is vital. MOR aims to reduce the computational burden by generating reduced-order models (ROMs) that are faster and cheaper to simulate, yet accurately represent the original large-scale system behavior. MOR replaces (3) by a ROM $\mathbf{E}_r\mathbf{x}_r' = \mathbf{H}_r\mathbf{x}r + \mathbf{f}_r(\mathbf{x}_r) + \mathbf{B}_r\mathbf{u}$, $\mathbf{E}_r\mathbf{x}_r(0) = \mathbf{E}_r\mathbf{x}_{r_0}$, $\mathbf{y}_r = \mathbf{C}_r\mathbf{x}_r + \mathbf{h}_r(\mathbf{x}_r)$, where $\mathbf{E}_r, \mathbf{H}_r \in \mathbb{R}^{r\times r}$, $\mathbf{f}_r \in \mathbb{R}^r, \mathbf{B}_r \in \mathbb{R}^{r\times m}$ and $\mathbf{y}_r \in \mathbb{R}^{\ell\times r}, \mathbf{C}_r \in \mathbb{R}^{\ell\times r}$, $\mathbf{h}_r \in \mathbb{R}^{\ell\times r}$ such that the reduced-order of the state vector $\mathbf{x}_r \in \mathbb{R}^r$ is $r \ll n$. A good ROM should have small approximation error $\|\mathbf{y} - \mathbf{y}_r\|$ in a suitable norm $\|.\|$ for a desired range of inputs $\mathbf{u}$. However, direct reduction of such systems leads to ODEs which are very difficult to simulate especially if the index of the DAE is greater than one. In [2], it was proved that DAEs arising from gas transportation networks are of index 1 if the gas network has only one supply otherwise they are of index 2. Thus, system (3) is of index 2. In [2], index reduction approach was proposed leading to ODEs which can further be reduced using standard techniques such as POD. However, this approach restricted on gas networks with special structure and leads to very stiff ROMs. We propose an index-aware approach which first automatically decouple the index-2 gas networks into differential and algebraic parts leading to ROMs which are also DAEs and easy to simulate.

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MS 09: Prognostic MR Thermometry for the Thermal Ablation of Liver Tumours

Efficient Therapy Planning via Model Reduction for Laser-Induced Thermotherapy

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We investigate the feasibility of pre-planning laser-induced thermotherapy treatments of tumours. The goal is to control the applied laser power in order to obtain an optimal treatment, e.g. eradicating the tumour, while leaving as much healthy tissue unharmed as possible. To this end, we define a PDE-constrained optimal control problem, which is computationally expensive. Therefore, we propose a simplified modelling approach using reduced-order models. Numerical results are presented in order to evaluate the viability of our methodology.

Validation of a Mathematical Model for Laser-Induced Thermotherapy

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A mathematical model for laser-induced thermotherapy (LITT) in liver tissue is validated. Simulated results are compared with experiments of laser ablation to ex vivo porcine liver samples. A laser applicator with internal water cooling and a temperature probe were inserted into a liver sample (see [1]). Radiation was applied and the temperature was measured during the whole experiment. The experiment was repeated for different laser powers and different flow rates of the cooling system. The experimental results are compared with simulated results. The mathematical model is based on [2] and consists of a system of partial differential equations, including the bio-heat equation and the P1 approximation for the radiative heat transfer. We present and discuss the experimental and simulated results and give an outlook of our ongoing research towards a planning tool for laser-induced thermotherapy.

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Improving Thermal Ablation of Liver Tumors

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Laser-induced thermotherapy is a medical treatment which attempts to destroy liver tumors by thermal ablation. A realistic real-time simulation shall support the practitioner online in planning the therapy. The heat transfer inside the liver can be described by a nonlinear coupling of the so-called bio-heat equation and a radiative transfer model. From a viewpoint of optimization, two interesting issues arise in this context. First, it is necessary to identify patient-specific parameters for the simulation using inverse methods. Second, it is worth investigating if, e.g., the duration of the therapy can be reduced by an optimized positioning of the laser applicator. In this talk we discuss first promising attempts to address these problems.

Acknowledgments The authors are grateful for the support of the German Federal Ministry of Education and Research (BMBF) grant no. 05M16UKE.

Mathematical Modeling for Laser-Induced Thermotherapy in Liver Tissue

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Laser-induced thermotherapy (LITT) plays an important role in oncology to treat human liver tumors. LITT is an alternative method which is used when surgery is too dangerous for the patient. It is a minimally invasive method causing tumor destruction due to heat ablation and coagulative effects of the tissue. Tumor tissue is much more sensitive to heat than normal healthy tissue. Most proteins denature at 40°C - 42°C. Irreversible coagulation necrosis occurs in the temperature range of 60°C to 100°C. LITT uses this effect. The big advantage of the LITT compared to other minimally invasive procedures, such as microwave ablation or radiofrequency therapy, is that the treatment takes place under MRI control using thermal sensitive MR sequences. Based on temperature-sensitive magnetic resonance parameters, such as proton resonance frequency, it is feasible to monitor the tissue temperature during cancer treatment (MR thermometry). Combining both MR thermometry and mathematical simulation is a promising procedure to identify temperature-depended tissue parameters and to optimize the cancer treatment. The present paper describes the mathematical modeling of the laser-induced thermotherapy. The well-known Pennes bioheat equation is coupled with the radiative transfer equation which describes the energy gain of the tumor tissue. The practical used laser applicator contains water cooling which has to be taken into account in the boundary condition for the heat transfer from the applicator into the liver tissue. Optical parameters (attenuation, absorption, and scattering) change due to thermal denaturation, which will be described mathematically by a damage function. We discuss the state of the art published in literature ([1, 2]) and present our model ([3]).

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MS 10: Mathematics of Planet Earth

Numerical Simulations of Drumlin Formation

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Drumlins can be loosely defined as small oval-shaped hills, generally occurring in large groups, that are found in regions once covered by ice sheets. They form part of a wider family of landforms known as subglacial bedforms, also consisting of ribbed moraine and mega-scale glacial lineations, whose formation is typically attributed to the motion of ice sheets. Despite attracting much scientific interest for well over 100 years [5], few quantitative descriptions elucidating the genesis of these bedforms have been proposed.

We summarise the present form of the instability theory of drumlin formation, which describes the coupled flow of ice, subglacial water, and sediment. The formation of subglacial bedforms is attributed to the linear instability of the model in which the preferred wavelengths for growth move continuously between regimes corresponding to ribs, drumlins, and lineations as a critical parameter is varied [4]. Thus the instability mechanism can naturally account for the self-organising behaviour observed in drumlin fields [1] and the hypothesized continuum of subglacial bedforms [2].

To investigate bedform evolution beyond the initial growth phase, we propose a novel numerical method to solve the model [3]. We demonstrate that simulations can be obtained for realistic values of most of the model parameters, with the exception of that corresponding to the water film thickness. Our results indicate that truly three-dimensional bedforms arise with sizes on the order of those observed in nature. One finds that these bedforms continually evolve in time and can resemble ribs, drumlins, and to a lesser extent, lineations.

Acknowledgments The authors are grateful for the financial support of Science Foundation Ireland under grant numbers SFI/13/IA/1923 and SFI/12/IA/1683.

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Great Balls of Fire - Modelling Surtseyan Volcanic Ejecta

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A Surstseyan eruption is a particular kind of volcanic eruption which involves the bulk interaction of water and hot magma. Surtsey Island was born during such an eruption process in the 1940s. I will talk about mathematical modelling of the flashing of water to steam inside a hot erupted lava ball called a Surtseyan bomb. The overall motivation is to understand what determines whether such a bomb will fragment or just quietly fizzle out.

Partial differential equations model transient changes in temperature and pressure in Surtseyan ejecta. We have used a highly simplified approach to the temperature behaviour, to separate temperature from pressure. The resulting pressure diffusion equation was solved numerically and asymptotically to derive a single parametric condition for rupture of ejecta. We found [1] that provided the permeability of the magma ball is relatively large, steam escapes rapidly enough to relieve the high pressure developed at the flashing front, so that rupture does not occur. This rupture criterion is consistent with existing field estimates of the permeability of intact Surtseyan bombs, fizzlers that have survived.

I describe an improvement of this model that allows for the fact that pressure and temperature are in fact coupled, and that the process is not adiabatic. A more systematic reduction of the resulting coupled nonlinear partial differential equations that arise from mass, momentum and energy conservation is described. We adapt an energy equation presented in G.K. Batchelor's book *An Introduction to Fluid Dynamics* that allows for pressure-work. This is work in progress.

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The Development of Deep-Ocean Anoxia in a Comprehensive Ocean Phosphorus Model

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The oceans and the underlying sediment represent major reservoirs of phosphorous. In order to fully understand the effect of anthropogenic alteration of the phosphorus biogeochemical cycle, an understanding of the oceanic component is necessary. Moreover, oceanic phosphorus is of particular interest because of the role it plays as a limiting nutrient over geological time scales. Slomp and van Capellen [1] studied the effects of oceanic mixing on phosphorus burial, and consequently on 'oceanic anoxia events'. These events mark periods (of hundreds of thousands of years) during which the deep ocean becomes anoxic [2].

The Slomp and van Capellen model describes the quantities of phosphorus, carbon and oxygen in different oceanic basins. Numerical results from their model indicate that mixing between these basins significantly affects the phosphorus cycle and deep-ocean oxygen concentrations. We show that this model can essentially be solved analytically, and its behaviour understood without recourse to numerical methods. Through non-dimensionalisation of the model equations and systematic simplification of the resulting system, we can distinguish oxic and anoxic regimes and the nature of the transition between them.

Acknowledgments We acknowledge the support of the Mathematics Applications Consortium for Science and Industry (www.macsi.ul.ie) funded by the Science Foundation Ireland mathematics grant 12/1A/1683. This publication has emanated from research conducted with the financial support of Science Foundation Ireland under Grant Number: SFI/09/IN.1/I2645.

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Production of Nitrate Spikes in a Model of Ammonium Biodegradation

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Microbial bioremediation is a process whereby naturally occurring bacteria in soil degrade, accumulate, or transform environmental pollutants. This counteracts groundwater contamination where plumes form from spills and leaks which develop locally and then migrate under the influence of groundwater flows. If these plumes reach streams, wells, or other sources of potable water then there can be serious risk to health.

Assessment of groundwater quality is often done using borehole biochemical analysis. One particular case study of this comes from Mansfield, U. K. where a rexco plant was discovered to have been leaking contaminants into the ground for decades. The site geochemistry was analysed by [1] and by the mid-1990s, the dominant contaminant remaining was ammonium. A borehole was dug and analysed ten years apart by [2] and [3]. The chemical and biological data from these analyses show emergent spikes in nitrate production as ammonium is utilised in both aerobic and anaerobic environments. This chemical transformation is concurrent with out-of-phase oscillations in two bacterial species which compete for ammonium as a resource.

In this talk we model nitrate production via a series of reduction-oxidation (redox) reactions mediated by bacteria in both aerobic and anaerobic regimes. We begin with a chemostat reactor model to show the presence of oscillatory dynamics and then incorporate spatial dynamics with diffusive processes and phreatic surface inputs. We demonstrate the presence of travelling waves and comment on the qualitative agreement with the data from Mansfield.

Acknowledgments This research is supported by grants from Science Foundation Ireland under grant numbers SFI/09/IN.1/I2645 and SFI/13/IA/1923. We acknowledge the support of the Mathematics Applications Consortium for Science and Industry (www.macsi.ul.ie) funded by the Science Foundation Ireland mathematics grant 12/1A/1683.

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A Model of Phosphorus Recycling at the Plant Scale

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Among the many crises facing humanity is the phosphate crisis [1], [2]. Four of the main essential nutrients for life are carbon (C), oxygen (O), nitrogen (N), and phosphorus (P) and the phosphate crisis stems from the fact that P is the only one of these nutrients that is not primarily sourced from the atmosphere. Instead, its availability is from very slow geophysical processes such as chemical weathering and soil formation from phosphate-bearing rocks. This source is unable to supply the needs of modern agriculture, which routinely uses fertiliser to satisfy the phosphate needs of crops. Understanding the mechanisms of P uptake and loss to the environment is important in preventing the overuse of this finite resource.

In this work we create a mathematical model of natural recycling of P through the surface accumulation of leaf litter in order to study the storage mechanisms of P on its overall cycle. Our model consists of mass conservation equations, written in terms of phosphorus content and include chemical processes such as chemical adsorption/desorption and biological processes such as phosphorus uptake by plant roots. The latter is presented using a Monod uptake term (cf. [3], [4]). The model has been solved by using matched asymptotic expansions and also numerically.

We will present results of the vertical profiles of P for soils with different phosphate sorption isotherms and address the following questions: How much crop can we harvest while still keeping the vegetative system alive? How will harvesting effect the fertiliser required to maintain the system?

Acknowledgments We acknowledge support from Science Foundation Ireland under grant number SFI/13/IA/1923.

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MS 11: Modelling of Cleaning and Decontamination

Chemical Decontamination with a Neat Agent and an Immiscible Cleanser

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When an oily chemical agent, such as mustard gas, has soaked into a porous medium, such as concrete, it can be difficult to neutralise using standard aqueous cleansers. The surrounding porous medium makes it difficult to promote good mixing, and the immiscibility of the agent and cleanser phases means that the decontamination reaction takes place at the interface between the two. In this talk, we develop and analyse a mathematical model for a decontamination reaction between a neat agent and an immiscible cleanser solution, where the reaction product is soluble in both the agent and the cleanser phases. The neutralisation reaction causes the interface between the two phases to move, and its location must be determined as part of the solution. We analyse our model using both asymptotic and numerical methods, and we investigate how different features of a cleanser affect the time taken to remove the agent. Our results reveal the existence of two regimes characterized by different rate-limiting transport processes, and we identify the key parameters that control the removal time in each regime. In particular, we find that the oil–water partition coefficient of the reaction product is significantly more important in determining the removal time than the effective reaction rate [1].

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A Model for Residue Removal in the Pharmaceutical Industry

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The cleaning of residues from equipment surfaces is a critical operation in the pharmaceutical industry. To prevent cross contamination of active produce ingredients (APIs), cleaning is performed during the changeover from the synthesis of one product to another. Cleaning has always been a time consuming and costly operation, but it has become even more problematic in recent years with an increasing focus on smaller production volumes resulting in increased numbers of product changeovers, and hence more time spent dedicated to cleaning. As a consequence, there is demand from industry to develop optimal strategies that minimise the time and resources spent on cleaning.

In this talk we outline a combined experimental and theoretical approach to explain the removal of a solid API from a surface via a cleaning solution. The experiment consists of a small-scale rig where a jet distributes a cleaning solution over an API on an inclined substrate. As the solution washes over the API and runs off, a UV-VIS spectrophotometer is used to infer the quantity of residue removed over time.

To explain the experimental results, we consider an advection-diffusion model consisting of the equations of motion and the diffusion equation for the API concentration in the solution. Dimensional analysis is used to highlight the relative importance of advection and diffusion with respect to API removal. The solution of the model is used to ascertain the key factors which affect the cleaning performance.

Acknowledgments The authors are grateful for the financial support of the Mathematics Applications Consortium for Science and Industry (funded by the Science Foundation Ireland grant no. 12/IA/1683) and the Pharmaceutical Manufacturing Technology Centre (an Enterprise Ireland & IDA Initiative).

Removal of Sulphur Dioxide from Flue Gas

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Gore's GMCS filter removes sulphur dioxide from flue gases by passing the gas through a filter comprising a porous structure made of sorbent-polymer composite (SPC) material. The gas adsorbs onto microscopic sorbent pellets in the SPC and reacts producing liquid sulphuric acid, which drains away along a network of fibres. Understanding the drainage mechanism and its driving forces is key to designing an effective filter. In this talk we consider a simplified problem of the surface-tension-driven spreading of a viscous fluid on a flat surface from part of the surface through which fluid is injected. This set-up is designed to mimic the production and accumulation of liquid sulphuric acid on a pellet within the SPC material and the subsequent drainage along a fibre. We use asymptotic techniques for a thin viscous layer to obtain power-law dependencies of the film thickness and the position of the apparent contact line on time, which agree with the numerical solution to the full problem. We also present a simple inverse problem for determining the time-dependent form of the injection rate by measuring the motion of the contact-line position. Finally, we show how we can couple this model to the diffusive mass transfer of the contaminant (sulphur dioxide), and how this affects the flow of the liquid film. Close collaboration with our partners at Gore enables our work to be tailored to the design challenge of sulphur-dioxide removal from flue gases and to more general applications involving spreading processes with injection of liquid.

Acknowledgements The authors are grateful for the support of the EPSRC fund and for the invaluable collaboration with W. L. Gore (Uwe Beuscher and Vasudevan Venkateshwaran).

Mathematical Modelling of the Decontamination of Chemical Droplets

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We study the decontamination process of small viscous droplets attached on a solid surface using a liquid decontaminant flowing over the droplets. This problem has applications in industrial cleaning, domestic dishwashers, and decontamination of hazardous material. First, we consider the decontamination of small droplets attached to an impermeable substrate inclined at an angle from the horizontal. During the decontamination, a liquid decontaminant is delivered onto the contaminated surface, forming a film flowing over the substrate under gravity. A combination of convection, diffusion and reaction processes govern the rate of decontamination, as the decontaminant film flows over the agent droplets. We investigate this problem through laboratory experiments, theoretical modelling and numerical simulations. We find that the Péclet number Pe of the film flow, which relates to the convective processes, has a stronger influence on the decontamination rate, characterised by the Sherwood number Sh, than the reaction rate, in the case of fully miscible polymer-thickened droplets with realistic reactant concentrations [1]. The mathematical model, which predicts a correction to the well-known relationship $Sh \sim Pe^{1/3}$, is in good agreement with experimental data.

In the second scenario, we investigate the decontamination of droplets which have migrated inside small gaps or cracks of a substrate under the effect of gravity or capillary forces. Building surfaces are often a composite of different materials with joints and gaps between them. The materials themselves (e.g. bricks, concrete, or mortar) can also have cracks, which can be much harder to decontaminate than external impermeable surfaces. We present the results of numerical and theoretical investigations of this problem. In particular, we find that the flow of decontaminant and the convective processes are limited by the confined geometry of the gaps and cracks. Depending on the details of the geometry and the Péclet number, we find different regimes where convective and diffusive processes have varying impact on the mass transfer and the corresponding Sherwood number. Our theoretical model is in agreement with the numerical simulations.

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MS 12: Networks in Finance and Social Sciences

Katz centrality, control analysis and directed networks

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Network centrality measures are used to identify the most important nodes that govern dynamics on networks. Effective identification of these nodes has applicability in, for example, social network structures, epidemic contact networks and biochemical networks. In this presentation I particularly focus on Katz centrality, first proposed by Leo Katz in 1953 [1]. Katz centrality is directly related to eigenvector centrality and to Google's PageRank algorithm which I also discuss.

I present a different interpretation of Katz centrality as a steady-state solution to a continuous-time dynamical system which I refer to as Katz dynamics. By applying a control analysis to Katz dynamics, a more detailed understanding of centrality on directed networks is obtained [2].

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Can One Hear the Shape of a Country?

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Language is evolving everywhere, all the time. As a result, people from different parts of a country may use their language in quite different ways. These locally distinct versions are called dialects, or just accents if the differences are subtler. To map this geographical variation, linguists draw lines called "isoglosses" which mark boundaries across which some linguistic feature (a word, a pronunciation, or an element of syntax) changes. We present a coarse-grained network model for the dynamics of these lines based the assumption that peoples' language use is based on their linguistic memory, acquired in the regions where they spend most of their time [1]. We will show that isogloss velocity is given by a modification of the Allen-Cahn equation for the motion of magnetic domain walls in condensed matter physics. This linguistic Allen-Cahn equation predicts that isoglosses are driven down population gradients, feel surface tension, and that their end points tend to collect in boundary indentations such as river mouths and bays. We show how these effects link the shape of a country to the geographical pattern of its dialect areas, matching the observations of linguists. We will also explore the effects of long range interaction networks and population mixing [2], and introduce methods for inferring linguistic networks from historical data.

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Qualitative Analysis of the Compact Pairwise Model for SIS Epidemic Propagation

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Spreading processes on networks are widely studied by using stochastic and dynamical approaches. The mathematical model of such a process, like epidemic propagation on a graph, can be formulated as a large system of linear ordinary differential equations. For real-world large graphs these master equations are beyond tractability, hence the system is approximated by simple non-linear differential equations, called mean-field equations [1]. One of these low-dimensional ODE approximations for simple SIS dynamics is the compact pairwise model [2], for which the detailed study of steady states and the global behaviour has not been carried out yet. We prove that there is a disease-free steady state (without infection) of the system and characterize its stability. Besides that, it is shown that the endemic steady state is unique and a general transcritical bifurcation theorem is applied to show that the endemic steady state is locally asymptotically stable. Finally, the global stability of the disease-free steady state is proved for a wide range of parameter values.

Acknowledgments The project has been supported by the European Union, co-financed by the European Social Fund (EFOP-3.6.3-VEKOP-16-2017-00002).

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Application of Branching Processes to Simon's Model

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The occurrence of size distributions governed by power-laws in a wide range of system is a well studied phenomena described by Zipf's law [1]. Simon developed a simple model based upon a random copying with innovation mechanism where an individual creates a new element at each time step which is either a new variant with probability μ or of the same type as a randomly chosen previously used element [2]. This model results in size distributions characterized by power laws with exponent greater than two, as originally observed in empirical data.

Recent literature has taken advantage of branching process theory to modelling spreading phenomena [3] and this talk will introduce our work on using similar theory to describe Simon's model. A sample process shown in figure 1 gives an insight as to why a branching process lends itself to model the popularity of the red 'word'. We calculate the (age dependent) distribution of probabilities in the model and show they exhibit exponential tails only when taking the popularities over all ages do we obtain the heavy tailed distributions originally derived by Simon.

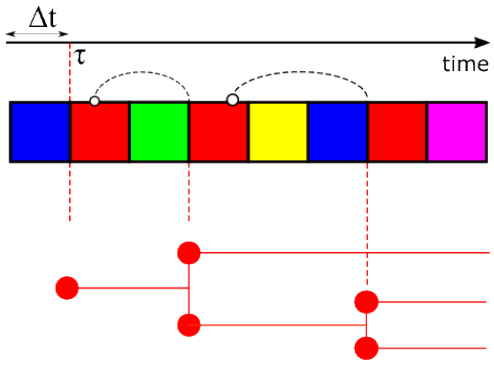

Figure 1: Simon's Model as a Branching Process

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Integrating Sentiment and Social Structure to Determine Preference Alignments: The Irish Marriage Referendum

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Twitter has been studied as an open and popular venue for the spreading of information and facilitation of debate. The accurate identification of the sides of a debate is fundamental to this. In this talk we will aim to answer the question: Is it possible to identify mutually positive and antagonistic relationships between groups, and understand how they interact with each other using network structure and sentiment? To this end, we examine the relationship between social structure and sentiment through the analysis of a large collection of tweets about the Irish Marriage Referendum of 2015. Using the sentiment of these tweets, we construct networks to aggregate sentiment and use it to study the interactions among users (Fig. 2). Our results show that the sentiment of mention tweets is correlated between users, and there are significantly more connections between users with similar sentiment scores than among users with opposite scores. Using this sentiment based homophily, we were able to classify users as either yes or no aligned supporters with high accuracy (89%). This allowed for the interactions of ideologically opposed users to be examined. For instance, there were numerous conversations between users on opposing sides of the debate in the absence of follower connections, which suggests that there were efforts by some users to establish dialogue and debate across ideological divisions. These results have potential applications in the integration of data and meta-data to study opinion dynamics, public opinion modelling, and polling.

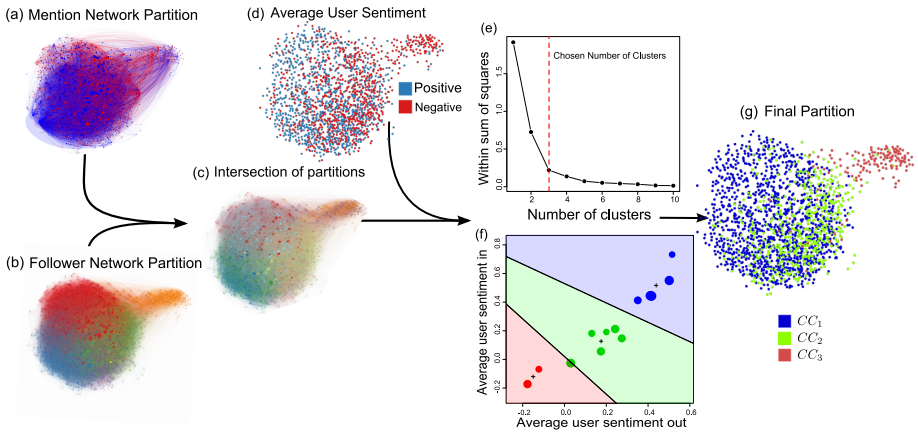

Figure 2: Schematic of our analysis of communities and sentiment. Communities in the mention network (a) follower, (b) networks and (c) their intersection. Mention network with nodes coloured according to sentiment (d). Sub-communities clustering according to their sentiment (e). Relationship between in- and out-sentiment of each sub-community and cluster membership is shown in (f).

Global Stability in Epidemic Models

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Propagation processes on networks have been widely studied by using the tools of dynamical systems. The main question, however, to relate the graph theoretic properties of the network to the dynamical behaviour of the induced dynamical system, has only been partially answered.
In this talk we consider a general dynamical system, where the right-hand-side function satisfies two assumptions. Our main result is that the global stability in this model can easily be verifed by a generalization of an idea of Lajmanovich and Yorke [1]. Using their idea, a global stability result can be proved for a quite general class of dynamical systems including the heterogeneous mean-field and the individual based mean-field models on a binary network process. As a by-product we will show that the same generalization can be applied to neural networks.

Acknowledgments The project has been supported by the European Union, co-financed by the European Social Fund (EFOP-3.6.3-VEKOP-16-2017-00002).

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Epidemic Threshold in Pairwise Models for Clustered Networks: Closures and Fast Correlations

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Networks have allowed to capture and model contact with an unprecedented level of detail leading to a major shift in how epidemics are modelled [1]. However, the propensity of contacts to clusters, e.g., neighbours of a node are also likely to be connected, continues to pose major modelling and analysis challenges. Apart from some theoretical results on idealised networks there are a limited number of general theoretical results. Mean-field models, such as pairwise models [2], have been used successfully in approximating the average behaviour of epidemics on networks and have led to significant results in terms of analytical epidemic threshold final epidemic size for susceptible-infected-recovered epidemics and networks with no clustering. While equivalents of the pairwise model for clustered networks are available there are limited analytic or semi-analytic results. In this paper we show show that it is possible to use the correlation structure at early times to work out a semi-analytic epidemic threshold using pairwise models for clustered networks. This is done by exploiting the difference in timescale of correlations versus that of the epidemic itself.

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MS 13: Modelling, Theory and Numerical Analysis of Reaction-Diffusion Problems

An Efficient 2D Arbitrary Lagrangian-Eulerian Modeling for Pulsed Laser-Matter Interaction

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The research on laser-matter interactions can bridge the gap between practical problems and applications of lasers, which offers an important way to study materials properties and to understand intrinsic microstructure of materials.

Laser-matter interactions are typically modeled by Lagrangian hydrodynamics as the Lagrangian computational mesh moving with the fluid is more suitable for the description of expansion or compression regimes appearing frequently in laser plasmas. However, many simulated problems in laser plasma (e.g. shear waves or physical instabilities) cannot be simulated by the pure Lagrangian method as the moving mesh degenerates with some computational cells becoming non-convex or even inverted. One can avoid mesh degeneration by employing Arbitrary Lagrangian-Eulerian (ALE) method [1, 2] which offers a possibility to avoid distortions of moving Lagrangian meshes. After several time steps of Lagrangian simulation or when the mesh becomes distorted, the deformed mesh is smoothed out by rezoning, the conservative quantities are conservatively remapped from the deformed mesh to the smoother one and Lagrangian computation can continue.

We have developed two-dimensional ALE code which is used to study the physical processes, the plasma absorption, the crater profile, and the temperature distribution on metallic target and below the surface. The mixed system of hyperbolic-parabolic partial differential equations is treated by splitting into hyperbolic and parabolic parts. The hyperbolic Euler equations are solved by the ALE method, while the parabolic heat equation is solved numerically by the proposed cell-centered finite volume scheme [3].

The results of numerical simulation of pulsed laser ablation are presented, and comparisons between experimental results and numerical ones are given which showed the robustness of our code. The study presents particular interest for the analysis of experimental results obtained during pulsed laser ablation.

Acknowledgments This work was supported by the National Natural Science Foundation of China (No.11571047 and No.U1730247).

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Cross-Diffusion Based Filtering. Applications in Remote Sensing

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An accurate study of the properties related to image processing of nonlinear initial and boundary value problems of 2×2 cross–diffusion type has been presented in [2]. The study includes among other subjects the well–posedness, a complete space–scale axiomatic, the existence of Lyapunov functionals, and the asymptotic behavior of the analytic solution.

On the other hand, the idea of introducing a linear filtering in satellite image classification prior to their classification has been successfully applied in [1]. In that work, a linear and nonlocal in time partial differential equation of diffusion type was considered at the filtering stage, leading to improve the results achieved by merely applying a classification procedure.

In the present work we show that a nonlinear cross–diffusion model (and local), instead of the nonlocal one commented above, at the pre–classification stage provides better final results in the image classification problems commented above. And not less important, by means of this approach the computer resources consumption is much less, in fact the memory requirement is greatly reduced as occurs with local models if compared to nonlocal ones and in particular with the one considered here. And of course the runtime is dramatically reduced as well, reduction which is even more noticeable if compared to other nonlinear classical models (e.g. anisotropic models) since the ones proposed in [2] do not require additional numerics for the diffusion coefficients.

A large variety of numerical illustrations will be presented, including the estimation of forest fire affected areas, or coal mining affected areas in several places located in the northern Spain. Several classical statistical indexes will be considered to reveal numerically the quality of improvements achieved by means of this procedures.

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MLMC for Stochastic Delay Differential Equations in a Biochemical Setting

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In this talk we present numerical solutions to biochemical stochastic delay differential equations (SDDEs) via Multi-Level Monte Carlo (MLMC) methods.

Delay differential equations are required in biochemical settings, as time delay is an intrinsic property of many biochemical reactions. They have been studied for two different types: non-consuming and consuming delay. Gene transcription and translation induce a non-consuming delay, i.e. a gene continues to exist even after the process of transcribing has finished. In comparison, molecule transportation is a prominent example for consuming reactions, where the reactant disappears at the beginning of the reaction and the end product only appears after a time delay in another section.

In contrast to deterministic modelling of high particle numbers in physics, in biochemical problems one is usually confronted with systems containing low to moderate particle numbers. This gives preference to a discrete stochastic modelling of the system. Therefore, the inherent delay property as well as stochastic fluctuations need to be taken into account. It is then possible to mirror the dynamics of a chemical reaction network (CRN) containing delayed reactions and to estimate the state of the system adequately. Consequently, the setting in this paper reformulates the standard Markovian jump model for CRNs and adapts it to delayed reactions.

We present an application of the computationally efficient MLMC method in the setting of biochemical stochastic differential equations with delay. In order to build this adequate, fast simulation framework, we reuse techniques invented for the extension of MLMC to the setting of continuous-time Markov chains [1]. Using this idea with a path simulation as in [2], we construct biased as well as unbiased MLMC estimators for the system state. We restrict ourselves to fixed time delays. Numerical results stress the efficiency of our algorithm compared to exact algorithms, as we find a sharp decline of computing time for a prescribed accuracy.

Furthermore, we believe that the algorithm can be easily extended to other problems based on delayed Markovian jump models.

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Modelling Time-Of-Flight Transient Currents with Time-Fractional Diffusion Equations

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Since the 1960's there is an increasing interest and research on organic semiconductors, due to their particular characteristics (transparency, flexibility, low cost), as a material for the fabrication of optoelectronic devices, such as organic solar cells, light emitting diodes and light emitting transistors. The charge carrier mobility μ of these materials is one of the main properties of interest and the Time-of-Flight (TOF) technique is one of the preferred methods to estimate it. In the TOF experiment, a transient current $I(t)$ through a thin layer of material sandwiched between two parallel electrodes is obtained, as a result of the motion of excess charge carriers generated by a laser or voltage pulse, under the influence of an externally applied electric field E directed normally to the electrodes. These transient currents usually exhibit an anomalous dispersive character ([2]) with two regions with power-law behavior, separated by the transit time t_{tr} : $\sim t^{-1+\alpha}$, if $t < t_{tr}$ and $\sim t^{-1-\alpha}$, if $t > t_{tr}$ with $0 < \alpha < 1$. An estimate for μ is calculated from t_{tr}, the instant when the two power-law curves intersect. Such behavior is attributed to the trapping of carriers, in localized states distributed in the mobility gap, for times τ, or waiting times, determined by a relaxation function $\Psi(\tau)$ with an asymptotic time dependence of the form $\Psi(\tau) \sim \tau^{-\alpha}$.

In this talk we will explore the use of fractional derivatives in these models, continuing the work initiated in [1]. We particularly focus on the numerical approximation of the involved problems. As it is known, the solutions of fractional differential equations usually exhibit singularities in the origin in time, and therefore, a decreasing of the convergence order of standard numerical schemes may be expected. In order to overcome this, we propose a finite difference scheme on a graded mesh, in which the grading exponent can be properly chosen, taking into account the singularity type. Numerical results are presented and discussed.

Acknowledgments L. Morgado wish to thank FCT through the project UID/Multi/ 04621/2013.

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Coupling Convection-Diffusion-Reaction and Telegraph Phenomena: Second Order Approximations

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In this talk we consider a two-dimensional convection-diffusion-reaction equation with a convective velocity depending on the solution, and the gradient, of a telegraph equation. This coupled system can be used to describe drug transport under the action of ultrasound ([1, 2]).

Our aim is to define a piecewise linear finite element method (FEM) for the convection-diffusion-reaction equation that leads to a second order approximation for the concentration with respect to a L^2-norm. To do that we first define a piecewise linear FEM for the acoustic pressure that allow us to compute a second order approximation with respect to a H^1-norm ([3]). This method is then coupled with a piecewise linear FEM for the concentration. The convergence analysis is presented under lower smoothness requirements. Numerical results illustrating the obtained convergence orders are presented.

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Numerical Methods for Level-Set Equations

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In this talk we present novel approaches for solving advection and diffusion level-set equations on uniform and general polyhedral meshes. The semi-implicit methods, like inflow-implicit/outflow-explicit, are used for the time discretization and cell-centered finite volume methods are employed for the spatial discretization. The application fields cover image segmentation, point-cloud surface reconstruction and motion of phase interfaces, e.g. in combustion.

MS 14: Shape Optimisation Methods with Applications to Biology and Industry

Shape Optimization of Liquid Polymer Distributors

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In the context of industrial fiber spinning liquid polymer is pressed from an extruder into an externally heated distributor, which directs it onto a spinneret plate. From there the fluid exits the geometry through capillaries and is spun into fibers, which are then further processed. A long residence time of the fluid within the distributor can cause material degradation, which results in the blockage of the capillaries or a reduction of the fiber quality.

The shape optimization problem of designing optimal distributors by controlling the wall shear stress has previously been studied by Leithäuser, Pinnau and Feßler in [1] and [2]. We compare this approach with the ansatz of solving an additional convection-diffusion-reaction equation for the residence time introduced by Józsa and Krámer [3]. Following the optimize-first-discretize-then procedure we derive the shape gradient of a suitable cost functional by computing the adjoint and present first numerical results.

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Shape Optimization for a Stochastic Objective Functional

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Shape optimization is an important tool to increase the reliability of mechanical components. The use of stochastic objective functionals is beneficial as the failure mechanism is usually described using stochastic models. Furthermore, stochastic objective functionals are smoother than, e.g., maxima of point stresses.

Ceramic is a material frequently used in industry because of its favorable properties. We follow the approach above by minimizing the component's probability of failure under a given tensile load. Since the fundamental work of Weibull, the probabilistic description of the strength of ceramics is standard and has been widely applied. Here, for the first time, the resulting failure probabilities are used as objective functions in PDE constrained shape optimization. To minimize the probability of failure, we choose a gradient based method combined with a first discretize then optimize approach. For discretization finite elements are used. Using the Lagrangian formalism, the shape gradient via the adjoint equation is calculated at low computational cost. Furthermore, we construct shape flows towards an optimal / improved shape in the case of a simple beam and a bended joint.

Relation Between Shape and Mechanics:
Multiscale Modelling and Analysis of Plant Tissue Biomechanics

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Analysis of interactions between the shape of a plant tissue, mechanical properties and chemical processes, which influence the elasticity and extensibility of plant tissues, is important for a better understanding of plant growth and development. The main feature of plant cells are their walls, which must be strong to resist high internal hydrostatic pressure (turgor pressure) and flexible to permit growth. It is supposed that calcium-pectin cross-linking chemistry is one of the main regulators of plant cell wall elasticity and extension. To analyse the interplay between the mechanics, microscopic structure, shape and chemistry we first derive microscopic models for plant biomechanics (on the level of plant cell walls and cell wall microfibrils) and assume that the elastic properties of the cell walls depend on the chemical processes (interactions between pectin and calcium) and chemical reactions depend on mechanical stresses within the cell walls (modelling the fact that the stress within the plant cell walls can break the load-bearing cross-links). To study the mechanical properties of plant tissues and interplay between mechanics and shape, the macroscopic models are derived using homogenization techniques. Numerical solutions for the macroscopic models will demonstrate the patterns in the interactions between mechanical stresses, shape of plant cells and chemical processes.

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Shape Optimisation with Nearly Conformal Mappings

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The design of shapes that are in some sense optimal is a task faced by engineers in a wide range of disciplines. Often this problem can be expressed as the minimisation of an objective functional over a set of admissible shapes. Classical objectives are the drag or lift of a plane, the downforce of a race car, the strength of a structure, or the efficiency of an acoustic device.

Shapes are often discretised using meshes. When updating the shape, we want to move the initial mesh instead of generating a new mesh, as the process of remeshing is costly.

In two dimensions conformal mappings are good candidates for mesh deformations as they keep angles constant and can easily be characterised by the Cauchy-Riemann equations. We propose a method that augments the inner-product and norm on a function space in a way that deformations that lead to stretched mesh elements are penalized. We can make use of this new inner-product both in first order methods (steepest descent, L-BFGS) as well as in second order methods (Newton) to obtain fast optimisation methods that automatically choose mesh updates that retain the mesh quality of the initial mesh.

We present an analytical result stating that in a certain limit the chosen mesh updates are conformal. Furthermore we show several numerical examples that illustrate the performance of the resulting optimisation methods for simple toy problems as well as classical problems in aerodynamic shape optimisation.

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Refinement of Surfaces of Industrial Objects

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In industry, high quality (Class A) surfaces are frequently applied. Such surfaces are e.g. car-body surfaces, or surfaces of hydraulic machines. The styling design of vehicle surfaces is based on physical (clay) models, however, the construction, detail design and manufacturing is performed using computerized systems (CAD/CAM). The quality of the surfaces of the computer model must be evaluated prior to manufacturing. For that purpose, sensitive methods were developed; these are mainly the evaluation of the shape and distribution of reflection lines or highlight lines. They are calculated as the surface imprint of a linear light source array placed above the surface. Correction of highlight lines is usually performed interactively by the designer, which is time consuming and inaccurate. In the paper, we propose a method to semi-automatically evaluate and improve the quality of the highlight line structures. The structures are evaluated by the pattern and the individual shape of the highlight lines. A comprehensive quality inspection can be carried out by the comparison of the highlight line structures of different light source and surface position settings. The uniform or smoothly changing highlight line pattern is essential for the high-quality highlight line structures. Following the inspection, the defective highlight line segments are selected and corrected. The correction is carried out in two steps. First, sequences of evaluation points are defined to quantify the error in terms of distance and angle functions. Next, by function approximation the corrected highlight points are calculated, and based on these points the corrected highlight line segments are constructed. The correspondence between the shape of the reflection lines and the surface parameters is highly complicated and strongly nonlinear. In the paper a genetic process is proposed for the computation of the surface parameters reflecting the corrected highlight line structure. Application of the method is demonstrated by the correction of the highlight line structure of several industrial (car-body) surfaces.

Upscaling Volume Expansions Due to the Sulfate Corrosion of Concrete

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In this talk I present a sulfate corrosion model of concrete intended to determine the change in thickness of a concrete/gypsum layer due to both chemical reactions in and material flux into the domain. The model was built within a continuous medium mixture theoretic framework and it takes into account the interplay between mechanical forces, bulk and surface reactions, domain changes and material influx. Mathematically, the sulfate corrosion model is a nonlinear coupled parabolic-pseudoparabolic system with Robin boundary conditions. Existence of solutions follows the classical route of Rothe's time-discretization method suitably combined with Gronwall's lemma as well as compactness results due to Rellich-Kondrachov and Lions-Aubin-Simon. The qualitative behavior of the solutions with respect to the parameters is investigated numerically. Concerning eventual large scale applications of a simplified version of the sulfate corrosion model, we apply an homogenization approach in the spirit of the papers by M. Peszynska and R. Showalter about the homogenization of pseudoparabolic systems. This is joint work with Fons van de Ven (Eindhoven, NL) and Adrian Muntean (Karlstad, Sweden).

Multiscale Dynamics of Bulk and Leading Edge in Cancer Invasion

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Recognized as one of the hallmarks of cancer, cancer cell invasion into tissue is a complex process that plays a key role in the growth and spread of cancer, culminating in metastatic spread (secondary cancers). One common aspect of all cancer progression is the secretion of matrix degrading enzymes (MDEs) by the cancer cells that modify or destroy the surrounding tissue or various components of extracellular matrix (ECM) and support local cancer cell invasion. In conjunction with MDE activities, increased cancer cell motility due to changes in cell-adhesion properties further exacerbates the invasion. Transmembrane calcium-dependent adhesion molecules (cadherins) interact with intra-cellular proteins, such as ?-catenin and give rise to adhesion junctions. Of particular importance in cancer invasion are the dynamics between the calcium-sensing receptor distribution and the calcium ions (Ca2+) from the ECM. In addition to cell-cell adhesion, the binding of various ECM ligands to cell-surface receptors (integrins) enables cell- matrix adhesion. Thus, processes occurring at a molecular (micro) scale give rise to processes occurring at the tissue (macro) scale, via processes taking place at the cellular (meso) scale.

Despite recent mathematical modelling advances [1, 2, 3], the understanding of the biologically multiscale process of cancer invasion remains an open question. In this work we introduce a novel multiscale moving boundary approach for cancer invasion that accounts for cell-adhesion in the context of the multiphase nature of the ECM dynamics. Distinguishing here between the fibres component and the rest of the ECM components and incorporating their multiscale dynamics within the new modelling approach, this framework connects the tissue-scale macro-dynamics with both the proteolytic cell-scale dynamics occurring at the tumour invasive edge and the micro-scale ECM fibres dynamic degradation and realignment occurring inside the tumour domain. The presentation of the new modelling framework, will be accompanied by details of the computational approach and a discussion of the numerical simulation results.

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A Robust and Efficient Adaptive Multigrid Solver for the Optimal Control of Phase Field Formulations of Geometric Evolution Laws with Applications to Cell Migration

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In this talk, I will present a novel solution strategy to efficiently and accurately compute approximate solutions to semilinear optimal control problems, focusing on the optimal control of phase field formulations of geometric evolution laws. The optimal control of geometric evolution laws arises in a number of applications in fields including material science, image processing, tumour growth and cell motility. Despite this, many open problems remain in the analysis and approximation of such problems. In the current work we focus on a phase field formulation of the optimal control problem, hence exploiting the well developed mathematical theory for the optimal control of semilinear parabolic partial differential equations.

Approximation of the resulting optimal control problem is computationally challenging, requiring massive amounts of computational time and memory storage. The main focus of this work is to propose, derive, implement and test an efficient solution method for such problems. The solver for the discretised partial differential equations is based upon a geometric multigrid method incorporating advanced techniques to deal with the nonlinearities in the problem and utilising adaptive mesh refinement. An in-house two-grid solution strategy for the forward and adjoint problems, that significantly reduces memory requirements and CPU time, is proposed and investigated computationally. Furthermore, parallelisation as well as an adaptive-step gradient update for the control are employed to further improve efficiency. Along with a detailed description of our proposed solution method together with its implementation we present a number of computational results that demonstrate and evaluate our algorithms with respect to accuracy and efficiency. A highlight of the present work is simulation results on the optimal control of phase field formulations of geometric evolution laws in 3-D which would be computationally infeasible without the solution strategies proposed in the present work.

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. All authors acknowledge 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 authors (AM, FWY, CV, VS) 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. AM is a Royal Society Wolfson Research Award Holder, generously supported by the Wolfson Trust.

MS 15: Electromagnetic Problems Arising in Industry: Modelling and Numerical Techniques

Fully Discrete Solution for Bean's Critical-state Model with Temperature Effects in Superconductivity

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In this talk, we discuss a hyperbolic Maxwell-type variational inequality with temperature effects arising from Bean's critical-state model in superconductivity. Here, temperature dependence is included in the critical current due to its main importance for realizing superconducting effects, as confirmed through physical experiments. We propose a fully discrete scheme based on the implicit Euler in time and a mixed FEM in space consisting of Nédélec's edge elements for the electric field and piecewise constant elements for the magnetic induction. Under a regularity assumption on the initial data and a specific setting of the initial approximation, we prove that the fully discrete scheme admits a unique solution satisfying the discrete Gauss law, which turns out to be the key point for our analysis. Hereafter, stability estimates for the zero-oder and first-order terms of the proposed approximation are investigated. Our main result is the strong convergence of the fully discrete scheme without any further regularity assumption. In particular, the convergence result yields the existence of a unique solution for the variational inequality obeying the physical Gauss law. Furthermore, a priori error estimates are investigated under an additional Lipschitz assumption on the critical current and the temperature distribution as well as a higher regularity assumption on the continuous solution. We close our talk by presenting some 3D numerical results, which in particular confirm the physical Meissner-Ochsenfeld effect in superconductivity.

Isogeometric Boundary Elements in Electromagnetism: Towards Industrial Application

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One of the major trends in modern numerics is Isogeometric Analysis, first introduced by Hughes et al. [1]. The isogeometric framework uses CAD-generated NURBS[1] geometries themselves as the geometry discretizations, eliminates any additional geometry error, and reduces the amount of necessary preprocessing prior to simulations. Moreover, with smooth spline spaces to discretize the approximate solutions, the number of DOFs[2] can be reduced significantly. However, isogeometric finite element methods require the NURBS mappings to be volumetric; and most CAD applications yield only representations of the boundary. Fortunately, the requirement of volumetric discretizations can be overcome by the utilization of boundary element methods. Since the introduction of so-called fast methods [2] one of the major drawbacks of boundary element methods (BEM), namely the dense matrices arising from the underlying integral equations, has been overcome. Since then, BEM has become a feasible tool for industrial applications, in particular due to its inherent suitability for the numerical solution of linear exterior and/or scattering problems, see e.g. [3].

This talk will give an overview on the concepts of fast boundary element methods within the isogeometric framework (IGA-BEM). Discussing first promising applications of IGA-BEM for scalar problems (Laplace- and Helmholtz-equation) [4] we will introduce the fundamental notions of IGA-BEM, and then continue to elaborate on their utilisation in electrodynamics (electric wave equation), including an overview on the required theoretical concepts and state-of-the-art numerical results for electric scattering problems.

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[1]Non-Uniform Rational B-Splines
[2]Degrees of Freedom

Optimal Voltage Control of Non-Stationary Eddy Current Problems

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We are interested in the analysis of controlled electric or magnetic fields in electrically conducting media.

Often electrical currents are considered as controls, while the control of electrical voltages has been only investigated in the time-harmonic case, thus resulting in a dynamical system of elliptic type. However, it is more realistic to control the electrical voltage in a time-dependent setting.

In [1], [2], [3] the optimal control of electromagnetic fields by the electrical voltage is considered. A vector potential ansatz is applied to convert the standard magneto-quasistatic Maxwell equations in a (degenerate) parabolic system.

We present a different formulation, in which the principal unknown is the magnetic field (subject to the curl-free constraint in the non-conducting region). The associated model for the electromagnetic fields is close to that proposed in [4]. We merge the ideas of [4] with both a specific approach aiming at reducing the complexity of the Maxwell equations for given voltages and some ideas of adjoining in [5].

We devise the weak formulation of the problem and prove that it is well-posed. Then we furnish the formulation of the optimal control problem, and the adjoint problem and the necessary optimality conditions are derived. Some remarks on numerical approximation are also included.

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High Order Divergence Free Finite Element Basis

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We present an efficient algorithm for the computation of a basis of the space of divergence free high order Raviart-Thomas finite elements. The algorithm is based on graph techniques. The key point is to notice that, with very natural degrees of freedom for fields in the space of Raviart-Thomas finite elements of degree $r+1$ and for fields in the space of discontinuous piecewise polynomial functions of degree r, the matrix associated with the divergence operator is the incidence matrix of a particular graph. By choosing a spanning tree of this graph, it is possible to identify an invertible square submatrix of the divergence matrix and compute easily the moments for fields in the space of Raviart-Thomas finite elements with assigned divergence. This approach extends to finite elements of high degree the method introduced by Alotto and Perugia in [1] (see also [2]), for finite elements of degree one. This approach is used to construct a basis of the space of divergence free Raviart-Thomas finite elements.

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A Mathematical Approach to the Dynamic Preisach Hysteresis Model: Analysis and Computations

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Hysteresis is a phenomenon which is widely observed in a variety of physical systems. It introduces a nonlinear and multivalued behavior in systems, making their modeling and control problematic. Even though the analysis and mathematical properties of the classical or rate-independent hysteresis models are known, this is not the case for dynamic models where current approaches lack a proper functional analytic framework which is essential to formulate optimization problems and develop stable numerics, both being crucial in practice. This work deals with the description and mathematical analysis of the dynamic Preisach hysteresis model. Toward that end, we complete a widely accepted definition of the dynamic model commonly used to describe the constitutive relation between the magnetic field H and the magnetic induction B, in which, the values of B not only depends on the present values of H but also on the past history and its velocity. We first analyze mathematically some important properties of the dynamic model and compare them with known results of the static Preisach model. Then, as an application, we consider the mathematical analysis and the computation of parabolic problems with dynamic hysteresis motivated by electromagnetic field equations. Under suitable assumptions, we show the well posedness of a weak formulation of the parabolic problem and solve the problem numerically. Finally, we report two numerical test in order to assess the order of convergence and to illustrate the behavior of the numerical solution for different configurations of the dynamic Preisach model.

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Analysis of a Transient Magnetic Model with Voltage Drop Excitations

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The topic of this talk is the mathematical and numerical analysis of a nonlinear transient magnetic model defined in a two-dimensional domain, with sources given in terms of the potential drops in conductors and the remanent fluxes of permanent magnets. This model arises, for instance, in the simulation of electric machines and, in particular, of permanent magnet synchronous motors. In this kind of devices, the magnetic core is usually laminated orthogonally to the direction of the currents traversing the coils, and eddy current losses are often neglected in permanent magnets. Both of these simplifications allow us to build a 2D transient magnetic model in a cross section of the device, obtained from the low-frequency system of Maxwell's equations, the stator coils being the only conducting part. These coils are generally composed by stranded wires carrying a uniformly distributed current density and we will focus in the case where the potential drops are given in them. As a consequence, the distributed magnetostatic model has to be coupled with a circuit equation, linking currents and voltage drops. We will give a first step towards the analysis of the genuine physical problem, as we do not consider the motion of the machine, what would lead to a much more difficult problem; see, for instance, [1].

Firstly, we will obtain an integro-differential problem arising from the coupling of the transient magnetic distributed model with the circuit equations relating currents and voltage drops in stranded conductors. To perform its mathematical analysis, the model will be written as a nonlinear system of implicit ordinary differential equations in terms of the currents traversing the coils, which are functions of time. The operator defining this system expresses the so-called flux linkages per unit length in the coils in terms of the currents traversing them, via the resolution of some 2D magnetostatic problems. The properties of this operator are deduced directly from results from [2]. To perform the numerical approximation of the continuous problem, we propose an Euler-implicit scheme for the ODE, combined with a finite element method for the approximation of the involved distributed formulation. We will obtain convergence results for the proposed numerical scheme, which will be illustrated by some numerical results.

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Temporal Homogenization of a Nonlinear Parabolic System

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Inspired by induction heating models where a heat equation with time-scale of order of 1 s is coupled with a diffusive Maxwell equation with a time scale of order 10^{-4} to 10^{-6} s I will discuss a two-scale model for a nonlinear parabolic system. Assuming a rapidly oscillating inhomogeneity with period ϵ for one equation we carry out a formal periodic expansion to obtain a homogenized equation coupled to a local in time cell problem. We justify the expansion by deriving an error estimate between the original and the two-scale model and conclude with some numerical simulations.

(Joint work with S. Lu and J. Yu, Fudan University, Shanghai.)

Acknowledgments The authors is grateful for the support of the European Union's Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No. 675715 (MIMESIS).

MS 16: Multiple Scales in Electromagnetic Devices - from Quantum Mechanical Effects to Circuit Simulation

Electrothermal Feedback Due to Light Absorption Induced Device Heating

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Characterization of devices made of organic semiconductors is severe limited by their low charge carrier mobility [3]. As a consequence, the prototypical semiconductor physics known from inorganic materials for decades is often hidden behind a resistive charge transport. A way out are so called "Suns-Voc" measurements where the open-circuit voltage is measured for various light intensities [1]. Thus, the charge carrier recombination inside the device can be investigated without any modification due to charge transport as no current flows. Here, we discuss the effect of light absorption induced device heating during such measurements [2]. The change of the quasi-Fermi level is then not only related to the light intensity but also to the light intensity dependent device temperature. The resulting pseudo current-voltage characteristic has an S-shaped negative differential resistance and can be understood by some kind of electrothermal feedback which allows to reveal important properties such as the energy band gap, the thermal resistance, the device temperature and helps to learn about the ideality factor at high light intensities. The described effect is related to semiconductor devices in general and applies independently whether it is a solar cell or e.g. a light-emitting diode as long as the device builds up an open-circuit voltage upon irradiation with light.

Acknowledgments The author likes to thank the German Research Foundation (DFG) for funding within the project "Electrothermal feedback in organic devices" (EFOD) (RE 3198/6-1).

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Simulation of Optoelectronic Devices:
From the Atomic Structure to Macroscopic Device Properties

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The performance of modern optoelectronic devices like LEDs are determined to large amount by the properties of the materials employed in their active regions. Tuning of the properties of the light emitting layers e.g. can therefore help to improve device performance, especially when approaching theoretical performance limits. Since in the experiment mostly macroscopic device characteristics like current-voltage curves, emitted light power or efficiency are directly accessible, the material-to-device optimisation can greatly benefit from simulation approaches including multiple scales. Such modelling allows to predict macroscopic device behaviour under consideration of microscopic or nanoscale details like the local atomic structure in the active device regions. Ideally, such a combined simulation approach should not sacrifice too much the computational efficiency of device scale models, but also retain enough details from lower scales in order to bring in a real and industrially relevant advantage.

Here, we will show examples of linking between semi-classical electronic transport models like drift-diffusion and atomistic tight-binding approaches in order to include the effects of alloy order and compositional fluctuations into device level simulation. Such simulations are of interest in particular for III-nitride based quantum well and quantum dot LEDs, where the role of alloy fluctuations and inhomogeneity is still under debate [1, 2, 3]. These simulations not only help to improve basic understanding of the connection between atomic scale structure and macroscopic device behavior, but they would also allow for targeted tuning of the atomic structure in order to optimize device performance. This could be achieved by coupling the model with inverse design or optimisation codes, and considering that semiconductor industries have a good knowledge on the correlation between growth parameters and resulting material structure.

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Spherical-Harmonics-Based Solution of the Boltzmann Transport Equation on Supercomputers

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We present the design of a semiconductor device simulator employing the spherical harmonics expansion method to solve the Boltzmann transport equation on supercomputers. While the method has already been demonstrated to simulate fully three-dimensional device geometries [1] within several hours at moderate resolution on a single workstation, our work provides the ability to obtain simulation results faster and at higher accuracy. As a consequence, our work will aid in a better understanding of various phenomena, for example avalanche breakdown [2], for which established macroscopic approaches are insufficient [3].

Acknowledgments The authors are grateful for the support of the Austrian Science Fund (FWF), grant P 29119.

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Generalised Elements for the Analysis of Field/Circuit Coupled Systems

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Electrical circuits are classically simulated with Modified Nodal Analysis (MNA), which describes the circuit as a graph with lumped parameter models approximating the behaviour of the devices contained in the circuit. This yields a system of Differential Algebraic Equations (DAEs) for which it is known that the index depends on topological characteristics of the circuit [1]. The index analysis is for example useful to estimate the the sensitivity of the problem with respect to perturbations.

Sometimes, a more detailed description of specific elements within the circuit is needed. Then, an in-space discretised Partial Differential Equation modelling the specific device is coupled to the MNA. The index of the new obtained system has then to be analysed separately.

The talk presents generalised elements that allow to classify the systems coupled to the circuit and are capable to state the coupled system's DAE index by only studying the topology of the circuit. Several cases of generalised elements arising from electromagnetic field descriptions [2] are presented.

Acknowledgments This work is supported by the **'Excellence Initiative'** of the German Federal and State Governments, the Graduate School of Computational Engineering at TU Darmstadt and DFG Grant SCHO1562/1-2

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Analog-to-Probability Conversion - Efficient Extraction of Information Based on Stochastic Signal Models

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In many applications of analog signal acquisition, only certain features of the signal are of interest, and the exact waveform is not important. For these cases a new concept is introduced to determine the desired features without full signal conversion. A signal model has to be set up that contains the desired features as parameters. The current state of information about these parameters is represented by a multivariate probability distribution, approximated by a Gaussian. A digital-to-analog converter (DAC) and a comparator are used as signal acquisition hardware in order to increase the information about the parameters. In contrast to conventional analog-to-digital converters (ADCs), which convert the full signal waveform, this approach reduces the number of comparisons to be done by the acquisition hardware. Therefore the energy consumption can be decreased.

The DAC generates a threshold value that is compared to the analog signal. For linear signal models, the threshold corresponds to a hyperplane dividing the space spanned by the model parameters. The comparator output then indicates in which half space the true parameters defining the input signal are located, and the probability distribution is set to zero in the other half space, which decreases the variance. After renormalization and approximation of the remaining distribution as a Gaussian distribution again, this procedure can be repeated iteratively until the model parameters are determined with the desired accuracy. A particular advantage of the method is that less desired accuracy can be assigned to parameters of minor interest to avoid taking unnecessary samples.

In order to cover nonlinear signal models, where the dividing hyperplane is replaced by a curved hypersurface, the concept of a Gaussian mixture is introduced. It approximates the total probability distribution as a weighted sum of several smaller Gaussian distributions, which are placed in a grid to cover the whole parameter space. For each of these Gaussian distributions the hypersurface can be approximated by a hyperplane. Therefore the same method as described above for linear signal models can be applied.

Besides the reduction of comparisons, another advantage of the described concept is that it provides a priori information about the next samples. Therefore the most efficient sampling time and comparison threshold can be chosen to maximize the expected reduction of the parameter variances in each iteration.

As a proof of concept a prototype of an ADC utilizing the introduced algorithm was successfully implemented using a Cypress PSoC 5LP. The described concept is especially useful in applications where the processor executing the algorithm and the sampling circuit can be separated and very low power consumption of the latter is required. One example is the measurement of biosignals in medical implants.

Model Order Reduction for Dynamic Thermal Models of LED Packages

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Thermal management is one of the key issues arising in designing light-emitting diode (LED) based luminaire products. Dynamic compact thermal models (DCTMs) are required to predict the thermal behaviour of LED packages fast and accurately in system level simulations. The European Delphi4LED consortium aims to develop multi-domain (electrical-thermal-optical) compact models. One of its targets is to develop a methodology to extract DCTMs that can handle multiple heat sources of LEDs.

This presentation focuses on the implementation of Krylov subspace based model order reduction (MOR) methods [4] in extracting DCTMs for LEDs. Various techniques for generating DCTMs exist in the literature, for instance, see [1, 2, 3, 5]. Most of them focus on the extraction of DCTMs using thermal RC-network optimization techniques. MOR methodologies based on Krylov subspaces are capable of handling MIMO (multi- input-multi-output) dynamical systems. Hence, such methodologies are suitable for LEDs with multiple heat sources and multiple dies. The approach of MOR consists of semidiscretising the system of partial differential equations (PDEs) describing the physics of LED packages in the spatial domain using a 3D CFD tool such as FloTHERM, leading to a system of ordinary differential equations (ODEs) in the time domain. This can then be handled by several MOR techniques, and reduced to obtain acceptable compact model representations of the behaviour.

The results presented in this paper show that the extraction of DCTMs using iterative rational Krylov is highly accurate for a set of benchmark problems developed within the Delphi4LED project.

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Asymptotic-Preserving Schemes for the Semiconductor Equations

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The semiconductor equations have been widely used to model electronic devices for decades. Many numerical techniques have been developed, especially for simulating the operation of silicon devices. The same set of equations can easily be extended to include atomistic defects which allows simulation of challenging problems related to device fabrication and predictive design. These systems exhibit drastic differences in time-scales, including drift-diffusion of electrons and holes, drift-diffusion of atomistic defects, ionization reactions between defects and charge carriers, and chemical reactions between different types of defects.

To handle these massive differences in scale efficiently, we will introduce asymptotic-preserving numerical schemes for simulating the semiconductor system. In this talk, we will mainly focus on a differential-algebraic equations framework for dealing with Poisson's equation and applications to the fabrication and long-term reliability of II-VI photovoltaic devices.

This is joint work with Igor Sankin and Dmitry Krasikov (First Solar) and Dragica Vasileska and Abdul Shaik (ASU) as part of the DOE Award DE-EE0007536.

Coupled Electromagnetic Field & Electric Circuit Simulation: Co-Simulation Benchmark and Convergence Analysis

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We consider coupled dynamical systems, see [1], of the form

$$\dot{u}(t) + b(u(t), t) = c_1(\dot{x}(t), x(t)), \qquad u(t_0) = u_0, \tag{4}$$

$$f(\dot{x}(t), x(t), t) = c_2(u(t)), \qquad x(t_0) = x_0. \tag{5}$$

The ordinary differential equation (4) reflects the spatially discretized electromagnetic field equations, see [2], allowing also nonlinear materials such as semiconductors. The differential-algebraic equation (5) describes the equations of a lumped circuit obtained by the modified nodal analysis, e. g. see [3]. The vector valued time dependent functions u and x comprise the electromagnetic field and circuit system variables, respectively. The right hand side functions c_1 and c_2 describe the coupling of both systems. Notice that the systems dimension may easily reach millions of unknowns whereby the dimension of u is magnitudes higher than of x.
We discuss the advantages and limits of both, monolithic and co-simulation, approaches. Whereas the monolithic solving of (4) – (5) requires an implicit numerical solving scheme, the co-simulation approach allows (4) to be solved explicitly, e. g. using the Leapfrog integration, see [2]. Considering the dimension of u as the bottleneck, the latter is preferred. On the other hand c_1 and c_2 have to fulfill certain criteria in order to guarantee convergence of the co-simulation approach, contrary to the monolithic one, which are highly correlated to the subsystems' topological coupling.
Some exemplary coupled benchmark systems are analyzed due to fulfilling the sufficient criteria for the Gauss-Seidel and Jacobi iteration scheme which are derived from [4]. Further, numerical results are presented and discussed with respect to convergence, number of iterations, speed and memory.

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MS 17: Distributing Challenges - Efficiency Versus Constraints on Networked Consensus and Optimization

Consensus and Its Efficiency with Wild or Mild Constraints

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In this survey talk we will get an overview about various questions on *consensus*, that is, the process working with a distributed algorithm on a network that will make the nodes of a network somehow agree on a value based on their initial input.

It turns out that there is a strong tie between the computational, communicational capabilities of the nodes and the functions that can be evaluated cooperatively this way [2] to be the consensus value.

The most general choice for the function to compute is the average of the inputs. Still, two fundamental questions remain, how effective the algorithm is and how fault-tolerant it is if network disturbances are to be expected.

There are strong results to find fast solution with certain constraints [1] and also to take on challenges in the network, for instance, asynchronous communication [3].

In the last part of the talk we will also discuss recent results which demonstrate that a certain asymmetry may speed up the consensus process.

Acknowledgments The author is grateful for the support of NKFIH (National Research, Development and Innovation Office) grants PD 121107 and KH 126505.

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Bounding the Convergence of Mixing and Consensus Algorithms

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We consider distributed algorithms for the dual tasks of mixing to a probability distribution and reaching consensus over the nodes of a graph. A wide string of protocols has been proposed towards accelerating the basic "random walk" scheme of averaging over the neighbors [1]. The speedup of these protocols ranges from constant factor up to exponential in the number of iterations - leaving the question open of what speedup should in fact be feasible.

We show that it is possible to prove non-trivial bounds on this speedup [2], only requiring that the corresponding protocol obeys a mild condition of invariance, namely, that the protocol leaves its limit state invariant. More specifically, we show that any such protocol requires a number of steps lower bounded by the inverse of the graph conductance, thus extending a bound which was only known for the case of Markov chains. The latter is derived from an isoperimetric inequality on the underlying graph, quantifying its connectedness. We combine this inequality with simulability results that follow from the locality of the protocols - results that build on ideas from trying to describe quantum mechanics with local hidden variables. Indeed, we show how the generality of our approach also allows to restrict protocols relying on quantum mechanics, such as quantum walks [3].

Finally we will discuss further relevance of our results to concepts such as finite-time consensus and inverse eigenvalue problems, and sets of SIA (stochastic indecomposable aperiodic) matrices [4].

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Path-Complete Positivity as a Generalization of Consensus

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In one of the most traditional models for decentralized consensus systems, agents make convex combinations of the value communicated by their neighbours at every time step, and the question is whether this process will lead to consensus. The 'neighbours' are defined by a graph topology, which may change over time.

The crucial property guaranteeing that such a system tends to consensus is *positivity* of this system. In our work [1], the notion of *path-complete positivity* is introduced as a way to generalize the property of positivity from one LTI system to a family of switched LTI systems whose switching rule is constrained by a finite automaton. In order to do so, we leverage the recently introduced *path-complete Lyapunov technique,* which had been initially introduced for guaranteeing another property, namely stability, of constrained switched systems [2, 3].

Finally, we propose an algorithm for the automatic verification of positivity of a switched system, and investigate the application of the property to consensus systems.

This is joint work with R. Sepulchre, F. Forni, and G. Berger.

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On Network Centrality, Influence, and Resilience

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In the study of network systems the notions of centrality, influence, and resilience are ubiquitous. In particular, network centrality measures aim at quantifying the relative influence of the different nodes and/or links on the network system. On the other hand, resilience refers to the ability of the system to absorb and adapt to changes both in the exogenous loads and in the interconnection structure, limiting the propagation of such perturbations and maintaining an acceptable evel of functionality. In this talk, we first introduce some models of network systems from the social, economic, and engineering sciences and show how different notions of centrality emerge in the characterization of their dynamic and equilibrium behaviours. Then, we present some recent results on influence optimization in social networks and on the resilience of eigenvector and Bonacich centrality measures to perturbations of the network structure. The talk is based on joint work with Prof. Fabio Fagnani of Politecnico di Torino, partly published in [1, 2] and partly based on unpublished material.

Acknowledgments The author is partly supported by the Swedish Research Council and Compagnia di San Paolo.

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MS 18: Simulation, Optimization and Uncertainty Quantification of Field/Circuit Problems for E-Mobility Applications

Iso-Geometric Analysis as a Tool for Simulating Electric Machines

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Classically electric machines are modeled by the finite element method (FEM). One drawback is that the solution of the fields only have C^0 continuity across the different elements. Moreover, the geometry of the machine can only be approximated by polygons. To overcome these issues, we propose the use of iso-geometric analysis (IGA) [1] for machine modeling. The use of CAD basis functions, such as B-Splines and non-uniform rational B-Splines, in IGA enables the exact representation of arcs in the geometry. The regularity at the mesh interfaces can also be increased, which results in smoother and more accurate solutions than in FEM.

The geometry of the machine is built up by patches, which are constructed by two dimensional B-splines basis functions. In the air gap the patches are non-conforming, which necessitates a domain decomposition technique. This is obtained by decomposing the full computational domain of the machine into two subdomains. One subdomain is associated to the stator and the other one to the rotor. They intersect in the air gap. At this intersection a harmonic stator-rotor coupling [2] is conducted. This coupling procedure is applied to model an electric machine.

It is found that the proposed method is a promising tool for modeling electric machines. The results for the quantity of interest are in good agreement with the results obtained using classical FEM. Furthermore the proposed method is 20 times faster [3].

Acknowledgments This work is supported by the German BMBF in the context of the SIMUROM project (05M2013) and the PASIROM project (05M18RDA), by the DFG (SCHO1562/3-1), by the 'Excellence Initiative' of the German Federal and State Governments and the Graduate School of CE at TU Darmstadt (GSC 233/2).

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Cosimulation Interfaces for Field/Circuit Systems and Hystersis Modeling

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Cosimulation is an ad hoc simulation strategy to simulate coupled problems, which reuses and couples dedicated solvers. But, for coupled DAEs, contraction constraints need to be satisfied to guarantee convergence, e.g. [1]. Moreover the speed of convergence depends on the coupling interface among other aspects.

Conventionally in field/circuit coupling, the systems are naturally split at the domain borders, i.e., one subsystem with the field model, the other subsystem with the circuit (network) description. With respect to cosimulation, the splitting can be enhanced for an improved convergence.

The aims of the talk are twofold. On the one hand, we discuss convergence rates for cosimulation as well as enhanced splittings for field/circuit coupling and their properties: R- and LR-splitting [2, 3]. One the other hand, our next step is to include further effects as hysteresis and heat. Therefore, Tellinen's (scalar) hysteresis model is revisited [4]. Furthermore, ideas to generalize this model to include temperature dependence are presented. The generalization follows an analogous approach as the original hysteresis description.

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Multimaterial Topology Optimization of Electric Motors Based on the Topological Derivative

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This talk is about the topology and shape optimization of an electric motor based on the topological derivative and the shape derivative. We propose a two-stage algorithm where, in the topology optimization part, we employ the level set algorithm [1] which is based on the topological derivative. In a post-processing step, we apply a shape optimization algorithm based on the shape derivative [2], starting out from the final design of the topology optimization stage. We show results for the optimization with respect to two materials (e.g. ferromagnetic material and air) and an extension to the case of three different materials (ferromagnetic material, air and permanent magnet material).

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Sparse Representations for Uncertainty Quantification of Coupled Problems

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Multiphysics modelling of electric circuits and devices yields coupled problems, which combine partial differential equations and differential algebraic equations. A spatial discretisation generates a single dynamical system. The physical or geometrical parameters of a coupled problem are often affected by uncertainties due to measurement errors or imperfections of an industrial production, for example. Uncertainty quantification (UQ) is performed by a stochastic model, where critical parameters are replaced by random variables.

We consider an output of the dynamical system as a quantity of interest (QoI). The QoI is expanded into a series with orthogonal basis polynomials depending on the random variables. The number of multivariate basis polynomials up to a moderate degree becomes large in the case of many random parameters. Nevertheless, there is often a sparse representation (or low-dimensional representation), where just a few basis polynomials are required for a sufficiently accurate approximation. On the one hand, ℓ_1-minimisation yields a small polynomial expansion, see [1], for example. On the other hand, a model order reduction allows for the identification of a sparse representation of a QoI both in linear dynamical systems [2] and nonlinear dynamical systems [3]. We investigate the potential of the sparse approximation for a sensitivity analysis in the context of coupled problems. Numerical results of a test example are presented.

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Exploring Parallel-in-Time Approaches for Eddy Current Problems

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For the efficient use of massively parallel supercomputers for applications in science and engineering new parallel algorithms are required. The idea of parallelizing in the time dimension and, thus, adding an additional layer of parallelism to a numerical algorithm has become an increasing popular way to tackle evolutionary problems. Starting with the seminal work of Nievergelt in 1964 [1], various approaches for parallel-in-time integration have been explored. One important aspect when choosing a time-parallel method is its intrusiveness, i. e., the effort one has to put into implementing the method when aiming at adding parallelism to an existing time-stepping code. There are only a few time-parallel methods that are non-intrusive. In this talk, we describe two of these approaches, the Parareal method [2] and the multigrid-reduction-in-time (MGRIT) algorithm [3] which applies multigrid in the time dimension, resulting in a massively parallel and optimal scaling method. Furthermore, we discuss the use of Parareal and MGRIT for the time-parallel solution of eddy current problems. Eventually, these methods will be applied in the numerical optimization of electrical machines within the industrial-driven research project PASIROM, funded by the German Federal Ministry of Education and Research.

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Convergence Analysis of Parareal for Systems with Discontinuous Inputs

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The Parareal algorithm [1] allows to solve time-dependent problems in a time-parallel manner. Its convergence rate for nonlinear problems was derived in [2] under the assumption of regular (smooth) inputs. In the present contribution we perform a convergence analysis of a modified Parareal method for systems, which involve discontinuous right-hand sides. Such situations occur, e.g., in power engineering when electric devices are supplied with a pulse-width-modulated signal. In order to develop the theory for such problems we propose to use a low-frequency smooth input for the coarse propagator, e.g., from Fourier analysis. The influence of the input reduction on the overall convergence rate of the algorithm is illustrated by the derived error estimate. Numerical verification complements the theoretical findings and supports the obtained error bounds. Furthermore, similarly to the recent results of [3] on Parareal for the eddy current problem, we applied our modified approach with reduced coarse dynamics to the simulation of an induction machine and compared its performance to that of the standard Parareal method.

Acknowledgments This work has been supported by the Excellence Initiative of the German Federal and State Governments and the Graduate School of Computational Engineering at Technische Universität Darmstadt, as well as by the BMBF (grant No. 05M2018RDA) in the framework of project PASIROM.

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Uncertainty Quantification for Real Time Operation of Electromagnetic Actuators

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Linear electromagnetic actuators are utilized as basic parts of a wide range of cyber-physical systems, ranging from manipulators and control elements in industrial applications or building automation to active damping element in electric vehicles. Innovation of electromagnetic actuators has then huge impact on the inovation of many technical fields. The important requirements for state of the art actuators are here (i) high dynamic response, (ii) low energy consuption, (iii) operation safety (iv) high releability and (v) embedded intelligence. Therefore, our long-term research objective are novel concepts of electromagnetic actuator controlled by advanced model-based algorithms.

The major goal of presented research and development will be model-based fault detection methodology for high-performance electromagnetic actuators. Proposed approach is based on forward uncertainty propagation for nonlinear multi-physical model to determine probability of faultless operation under aleatoric and epistemic uncertainties. Afterwards, obtained results are used by control algorithm to make decision on occurred fault by fast calculation of reduced model.

Whereas, forward uncertainty propagation for nonlinear multi-physic model requires time-consuming numerical solution of coupled partial and ordinary differential equations, reduced model takes advantage of magnetic flux linkage precalculation on irregular grid of a multidimensional parameter space. The parameter space is than interpolated by multivariate algorithm and all required quantities for reduced model described by ordinary differential equations are calculated directly from the characteristic of the magnetic flux linkage. Proposed approach allow to balance computational effort of the algorithm with complexity of computational problem and then enables efficient solution of multi-physical model for controller and state observer of the system.

Acknowledgments This research has been supported by the Ministry of Education, Youth and Sports of the Czech Republic under the RICE – New Technologies and Concepts for Smart Industrial Systems, project No. LO1607.

MS 19: Control Charts and Case Studies

Risk-Based Control Charts in Process and Project Management

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Control charts are widely used tools not only in statistical process control (SPC), but nowadays also in project management [1]. Most of the control charts disregard the arising risks during the control procedure. Nevertheless, the monitored characteristics can be distorted by different sources like measurement error in production management [2] and estimation uncertainty in the field of project management. Ignoring measurement or estimation uncertainty can increase the cost of decisions. In this study, the authors show how to develop a risk-based control chart allowing to control both industrial processes and projects in order to reduce the decision costs.

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Generalizations of Cost-Optimal Control Charts for Healthcare Data

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In an earlier paper Zempléni et al. [1] introduced a Markov chain-based method for the economically optimal design of Shewhart-type control charts originating from Duncan's cycle-based model [2]. Recently, we developed this Markov chain-based approach into a method, which is suitable for real-life medical applications. In this model not only the shift size (i.e. the degradation of the patient's health) can be random, but the sampling interval (i.e time between visits) and the effect of the repair (i.e. treatment) too.

So far only the expected cost per unit time was considered as a comparison base between different control chart setups. The variance of this cost and its dependence on the different parameters can play just as - or even more - important role from the process control viewpoint. Motivated by this, we introduce a target function to be minimised, which incorporates both the average and the variance of the cost. The results are investigated using a purpose-built simulator - in this way one can e.g. test the variability of the costs. We demonstrate the usefulness of the approach for real-life data of patients treated in Hungary.

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Metamodels to Support Industry 4.0 in Glass Construction

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Easy to use without expert knowledge - such a planning tool saves time and money. This talk introduces a new and efficient calculation option, which enables sales staff or architects to quickly check if a chosen all side supported glass pane is resistance to a soft body impact at an early stage of planning. It is demonstrated, how a metamodel generated on simulated data and adapted to the type of product can be used to ensure a reliable, automated and quick evaluation of the specific client preferred product parameters to guarantee the demanded characteristics of the final product without consultation of human expert knowledge.

Data Science in Industry 4.0

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Data science is piquing the interest of many large and small organisations and managers are asking universities for information and advice. Typically, the query is: I have many sensors and many measurements, what shall I do with all this data, and how can I get ready for Industry 4.0? The so-called 4th industrial revolution refers to automation and control based on data exchange in a digital environment where measurements are available on all aspects of production. Data science plays an intrinsic role in this scenario and is focused on understanding and using data. Data science requires a challenging mix of capability in data analytics and information technology, and business know-how. Statisticians need to work with computer scientists; data analytics includes machine learning and statistical analysis and these extract meaning from data in different ways. Moving towards increased use of data requires buy in from higher management and board members. Although serious progress involves a holistic approach, exemplars demonstrating potential value are also beneficial. This talk considers the implications for mathematicians and statisticians of the growing industrial demands and discusses examples from ongoing research projects with industrial partners where data visualisation, multivariate statistical process control charts and funnel plots have made an important contribution.

MS 20: Differential Equations and Optimisation

Production Network Models with Stochastic Capacities

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We focus on production network models based on coupled ordinary and partial differential equations combined with time-dependent random capacity functions. The partial differential equations are scalar conservation laws and of hyperbolic type coupled with ordinary differential equations at the boundaries.

In a first step, the random capacity function of every processor is an external given stochastic process, a semi-Markov process that allows intermediate capacity states in the range of total breakdown to full capacity. The operating and down times can be arbitrarily distributed, provided they keep positive. The mathematical challenge is to combine the theory of semi-Markov processes within the framework of conservation laws and the solution concept [1].

In general, the assumption that capacity drop probabilities are independent of the production and external given by a stochastic process is too restrictive. A high workload implies a high abrasion or stressed working conditions whereas an empty production is not affected by capacity drops for example. This motivates to introduce an influence from the production to the capacity process as well and we obtain a bidirectional relation between the production and the random capacity process. For this purpose, we define the stochastic load-dependent production network model as a stochastic process in a whole and embed it into the theory of piecewise deterministic Markov processes [2].

We present solution concepts for both stochastic production network models and show the well-posedness. Caused by the complexity of the model, we state suitable simulation methods and performance measures to evaluate and interpret the results. A variety of numerical examples emphasizes the characteristics of the proposed approach.

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Bayesian Parameter Estimation for Macroscopic Pedestrian Dynamics Models

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The fundamental diagram of pedestrian dynamics relates the experimentally observed density of pedestrians to their average velocity. Although there is a general agreement on its basic shape, its parametrization depends strongly on the measurement and averaging techniques used as well as the experimental setup considered.

We aim at developing a systematic approach to identify parameters in nonlinear macroscopic crowd motion models using multiple microscopic trajectories. We assume that each trajectory is a realization of an Ito-McKean process, where the individual velocity depends on the probability density of the process. The probability density satisfies a nonlinear Fokker-Planck equation itself, leading to a coupling between the microscopic SDE and the macroscopic PDE.

Motivated by the fundamental diagram we assume that individuals move with a maximum velocity, which decreases linearly as the probability density approaches the maximum crowd density. We are interested in identifying the maximum velocity and the maximum crowd density using multiple trajectories. We discuss Bayesian as well as other derivative free optimization methods to estimate these parameters and present analytic as well as numerical results, which give important insights into the dynamics and challenges of this highly nonlinear inverse problem.

Guiding a Huge Crowd by Controlling Few Leaders

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We discuss a huge ODE system modelling a crowd of self-organizing individuals and few leaders. In order to control the system, i.e. steer the crowd to some predefined destination, we set up an optimal control problem and derive the first order optimality system. Due to the curse of dimensionality we are interested in a reduction of the system and consider therefore the mean-field limit of the particle system that models the crowd. This raises several questions: Do the controls of the ODE system converge to the mean-field controls for $N \to \infty$? Do the results change if we interchange the order of computing the adjoints and passing to the mean-field limit? Can we reduce the computational cost of the optimization by using instantaneous control or feedback control strategies? Can we extend the results to SDE systems? We discuss these questions and underline the theory by numerical results [1].

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Modeling and Simulation of Macroscopic Pedestrian Models

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We analyze numerically some macroscopic models of pedestrian motion such as Hughes' model [1] and mean field game with nonlinear mobilities [2] modeling fast exit scenarios in pedestrian crowds. A model introduced by Hughes consisting of a non-linear conservation law for the density of pedestrians coupled with an Eikonal equation for a potential modeling the common sense of the task. Mean field game with nonlinear mobilities is obtained by an optimal control approach, where the motion of every pedestrian is determined by minimizing a cost functional, which depends on the position, velocity, exit time and the overall density of people. We introduce mean-field limit to the microscopic setup of optimal control problem which leads to a parabolic control problem and the optimal conditions gives a mean field game structure for pedestrian flow. We show how optimal control problem related to the Hughes' model for pedestrian motion. Furthermore we provide several numerical results which relate both the models in one and two dimensional cases.

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Equilibrium, Stability and Shape Optimization
Nonlinearly Elastic Corrugated Membranes

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The paper presents a numerical-analytical algorithm for determining branch points for circular membranes with an arbitrary profile along the meridian. This class includes a large number of corrugated membranes used as elastic elements in precision mechanics [1, 2]. A spherical dome with possible deviations from an ideal surface can be considered as a special case. To describe the large elastic strains of the membrane under hydrostatic pressure two-dimensional nonlinear equations [3], based on the Kirchhoff's hypotheses, were used. Some questions of numerical integration of a nonlinear boundary value problem for the sixth order ODE system for the analysis of the axisymmetric deformation are discussed. A linearization scheme for the initial non-axisymmetric boundary value problem for determining branch points of its axisymmetric solutions and a numerical scheme for searching for bifurcation points are described. Two approaches are presented for studying the post-critical behavior of a membrane.

As a first example of an application of the developed theory a problem of shape modulation of a spherical dome was investigated. It was established that the points of local maximum and minimum, if any, on the pressure-displacement diagram in the axisymmetric case are bifurcation points. It is shown that the experimentally manifested sensitivity of a spherical dome to imperfections is associated with a large number of closely located bifurcation points along non-axisymmetric modes. By deliberately introducing small technological changes in the shape of the dome, it is possible to eliminate most of these bifurcation points to ensure the operation of the shell in an axisymmetric mode.

As a second example of the use of developed techniques for analyzing the equilibrium and stability of corrugated membranes, a number of problems of optimal membrane design have been considered. Optimization of the shape of corrugation was carried out using a genetic algorithm. Calculations have been carried out to prove its effectiveness.

Acknowledgments The research is partly supported by a grant from the Vladimir Potanin Charity Fund (project GPK-96/17). The results of the study will be used in the Master Program Computational Mechanics and Information Technologies.

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Optimization of Buckling Behavior for Textiles

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The problem comes from companies using thin and slender strip-type textiles (carrying straps, safety belts, etc.), that come to a buckling under tension. This buckling occurs in the direction perpendicular to the tensional one. The goal for the companies is the reduction of such buckling phenomenon, since it can lead to critical effects.

Hence, the mathematical task is devoted to the optimization of the textile structure, in order to reduce the buckling. The objective functional is so either delay of the first buckling mode or the reduction of its amplitude. Both depend on the effective material properties of the textile, then seen as thin sheet, and the applied tensional forces.

However, the preliminary modeling step is to understand the textile itself and to decide, which macroscopic characteristics are important, how the can be computed from the yarn's properties and the textile pattern and also an idea where a change in design is possible. The homogenization theory gives a way to pass from a periodic woven fiber-structure of the textile, to a macroscopic shell model, able to recover the buckling behavior.

For instance, the von-Kármán-model is capable to model a buckling or wrinkling by the loss of coercivity for certain choice of parameters and forces. In this case the equation is not uniquely solvable anymore, but the solution can be represented as a combination of corresponding eigenvectors. Eventually, an optimization can be applied, which covers the maximization of the eigenvalue (delay of the first buckling) and/or a modification of the first eigenmode to stay closer to a flat shape (amplitude reduction).

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MS 21: MSO4SC: an Infrastructure for MSO Frameworks and Software

Reservoir Simulation Using the MSO4SC Infrastructure and OPM Flow

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The "Modeling, simulation, optimization for societal challenges" (MSO4SC) project aims to provide mathematical technology as a service through an HPC-oriented e-infrastructure [mso4sc.eu]. The goal is to lower the barrier to using MSO software, which otherwise typically requires a wide range of expertise, including knowledge of the problem domain, numerics, programming, parallelization, databases and visualization; some or all of which may not be available to decision makers or industrial actors. In this talk we discuss some of the results from this project with respect to the Open Porous Media (OPM) framework.

The OPM software is an open-source collection of software modules for porous media applications [opm-project.org], from which one can construct a range of simulators for porous media problem. OPM is a collaborative effort. It involves research institutes such as SINTEF, IRIS and TNO; industrial companies like Statoil, and universities. Open data sets and a visualization tool is also provided under the OPM umbrella. One important goal of the OPM initiative is to create software that is industrially relevant in terms of capabilities and performance and at the same time useable as a basis for academic research. This benefits both researchers, who can test new methods and algorithms on real industrial problems, and industry, which more rapidly can take advantage of advanced methods from research. OPM is one of the mathematical frameworks that are part of the MSO4SC project.

The reservoir simulator OPM Flow is one of the pilot applications of MSO4SC. In reservoir simulation, simulating ensembles of cases is of particular interest. It is often useful to run multiple realizations of cases to account for uncertainty in the underlying physical properties, such as permeability. We discuss how an early version of the MSO4SC infrastructure has been used for ensemble studies of reservoir production optimization, using the OPM Flow pilot.

MSO4SC: Cloud E-Infrastructure Designed by and for the Mathematical Community

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Development and usage of MSO (Modeling, Simulation and Optimization) software normally involves several areas of expertise, not only those directly related with MSO but also HPC (High Performance Computing). The MSO4SC Project (Modeling, Simulation and Optimization for Societal Challenges with Scientific Computing) intends to significantly ease the usage and deployment of MSO software and to hide the underlying complexity of the computational resources by means of the MSOcloud.

The MSOcloud is an e-infrastructure that provides, in a user-driven, integrative way, tailored access to the necessary services, resources and even tools for the fast prototyping and to reduce time-to-market, providing the service producers with the mathematical frameworks as well. The e-infrastructure consists of an integrated MSO applications catalogue containing models, software, validation and benchmark as well as an experimentation tool for facilitating simulations execution. The platform supports heterogeneous, HPC and multi-cloud systems and is designed taking into account the optimal provisioning configuration of the main mathematical application classes: distributed memory (MPI), shared memory (OpenMP) and embarrassingly parallel.

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High Field Magnets Design and in Operation Toolchain in the Cloud with Feel++ and MSO4SC

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High Field Magnets are an essential ingredient for many research area (e.g., High Energy Physics in CERN, High-resolution MRI for neurosciences, New material like Graphene or High-Temperature Supraconductor). The Laboratoire National des Champs Magnétiques Intenses (LNCMI) is a French large-scale facility [1], also part of the European Magnetic Field Laboratory (EMFL), that provide access to such magnets in solenoidal configuration up to 37 T static field and 99 T pulsed field for the international scientific community. At LNCMI, the static fields are provided by water-cooled resistive magnets connected with a 24 MW power supply.

In a strong international competition driven by the NHMFL (USA), the LNCMI is embarked into the race for a higher field. To keep up with this context magnet technologies have to be pushed to their limits both regarding materials (active researches are carried out to have materials – either resistive or superconductor – with improved mechanical and electrical properties) and design methods. The HiFiMagnet project, carried out in collaboration with Cemosis [2, 3] at the University of Strasbourg, had been developed to tackle these challenges. It aims at (i) providing a hierarchy of numerical models ranging from 2D-axi to 3D, and including more and more physics, (ii) complementing our standard design by performing sensitivity analysis and uncertainty quantification on material properties, operational parameters, and geometric clearances. Our objective is to improve our standard design and optimization procedures by providing complete and powerful modeling.

In this talk, we present the HiFiMagnet contribution to the European project MSO4SC[5]. We bring the Hifimagnet software toolchain for solenoidal magnet - based on *Feel++*[4] framework - to the magnet designer. Our goals are (i) to provide more precise multi-physics simulation, (ii) to identify the important parameters, and (iii) to perform quantile estimation and compute the probability of failure for safer operational controls.

Acknowledgments This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 731063.

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[4] http://www.feelpp.org

[5] http://mso4sc.eu/

Mono- and Multi-Physics Toolboxes in the Cloud with Feel++ and MSO4SC

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Feel++ is a Finite Element method Embedded Language written in C++ [1] to solve partial differential equations using standard Galerkin methods. Feel++ provides a mathematical kernel that encompasses a broad range of numerical methods such as (i) arbitrary order continuous and discontinuous Galerkin methods in 1D, 2D, and 3D, (ii) domain decomposition methods, (iii) fictitious domain methods, (iv) level-set methods and (v) reduced-order methods.

In this talk, we present the Feel++ Toolboxes which were introduced in the framework to solve mono- and multi-physics problems encountered in research fields such as health, physics, mechanical engineering. The toolboxes are built with ease of use in mind and are programmable with C++ and Python. Thanks to container technologies, Docker and Singularity, we provide a robust environment with Continuous Integration (CI) and Continuous Delivery (CD) for Feel++ and its associated projects. The Feel++ containers comprise a complete programming and runtime environment, from pre- to post-processing to allow basic to advanced Feel++ usage. A benchmark framework is being developed to improve reproducibility. It generates automatic versioned descriptions of test cases or benchmarks with the prospect of better documentation. We shall emphasize how we adapted Feel++ and its toolboxes to deploy them in the HPC/cloud EU H2020 e-infrastructure MSO4SC [2].

Acknowledgements This project has received funding from the European Union's Horizon 2020 research and innovation program under grant agreement No 731063.

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The FEniCS-HPC High Performance Finite Element Framework and an Adaptive Turbulent Flow Solver Application in the MSO4SC Project

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In this talk we present the Finite Element Method (FEM) Framework Fenics-HPC, and discuss an adaptive turbulent flow solver with a Direct FEM Simulation Methodology. The incompressible Navier-Stokes equations are solved numerically in an approximation space of piece-wise linear polynomials on conforming tetrahedral meshes with additional least-squares based stabilization terms. The mesh is adaptively refined with the solution of a dual problem acting as weights on the residuals.

The results on example validation cases such as time-dependent turbulent flow around an aircraft in full landing configuration from the 3rd AIAA High Lift Prediction Workshop and Tandem Spheres Re=3900 test case from the 5th International Workshop on High-Order CFD Methods will be presented.

Another discussion point will be the continuous integration component of the framework with test cases controlling not only the accuracy but also parallel scaling properties. This component is implemented in the context of the MSO4SC project (Mathematical Modelling, Simulation and Optimization for Societal Challenges with Scientific Computing).

Molecular Simulation for a Successful Computational Drug Design (ZIBAffinity)

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As described in [2], predicting interactions between small drug-like molecules and clinically relevant target proteins is possible by using computer simulations of host-guest systems on a classical atomistic level. ZIBAffinity is a corresponding simulation software which runs on HPC machines. With the aid of molecular simulations it was possible to invent a new pain-relief drug candidate that it urgently needed, e.g., because of the opioid crisis in USA [1]. We will present the role of molecular simulation for societal challenges and the integration of a software like ZIBAffinity into a platform like MSO4SC.

Acknowledgments The authors are grateful for the support of the H2020 project MSO4SC.

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Next Generation Markov Modeling for Protein Function Design (GenPCCA)

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Molecular simulations require a vast amount of computational power due to its high dimensionality and complexity. One possibility to treat this problem is to describe the molecular system in terms of evolution of probability densities governed by some (e.g. Fokker-Planck) operator. In Markov state models (MSM) a suitable Galerkin discretization of this operator is employed such that the systems dynamics can then be described by a Markov chain. Typically this Markov chain is still to large, therefore the eigenvalues and eigenfunctions of the corresponding Markov transition matrix are used to span an invariant subspace, where the system can be described in a coarse grained manner. For spanning such an invariant subspace it is often required, that the underlying Markov chain is reversible. Here, we present a novel method, which does not need this assumption by still providing such a coarse scaled description. We also give examples from the simulation of biomolecules and eye tracking data, showing the performance of this novel method.

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MS 22: Mathematical Modelling of Industrial Processes

On Dry Spinning Processes In Airflows

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During dry spinning processes solvent evaporates out of the spun jets and leads to thinning and solidification of the final fibers. In industrial dry spinning processes multiple fibers are spun simultaneously, such that the whole process is significantly driven by the interaction of the fibers with the surrounding airflow. Due to these multiphase and multiscale effects the three-dimensional simulation of this problem is computationally extremely demanding. Therefore, we propose an efficiently evaluable dry spinning model: We describe the fiber dynamics by a one-dimensional uni-axial viscous two-phase flow resulting from cross-sectional averaging of underlying three-dimensional balance laws. To include radial effects, observable in experiments, we propose an iterative coupling with consistent two-dimensional advection-diffusion equations for solvent concentration and temperature, which can be solved very efficiently in terms of Green's functions and employing the product integration method. These efficiency allows further coupling with the surrounding air based on the action-reaction-principle.

Microwaves Measure Moisture — mmm, Really?

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Measure the moisture content of bauxite in real time on a conveyor belt as it is offloaded from a ship - this is the challenge that alumina company Rusal Aughinish brought to a European Study Group with Industry, held during one week in June last year at the University of Limerick in Ireland. Rusal are using a recently installed microwave analyser, and they sought our judgement on the reliability of the moisture measurements produced by the analyser. If you come to this talk, you will hear how we tackled the data and information provided, and what we learned about the physics of microwaves propagating through a field of polarisers. There will be some data science and some data hygiene, there will be some insight into how noise affects phase shift measurements, and there will be evidence of interference between reflected and transmitted waves. Come, find out what a squircle is, and be amazed at the twist and turns of our negotiations of the path to enlightenment.

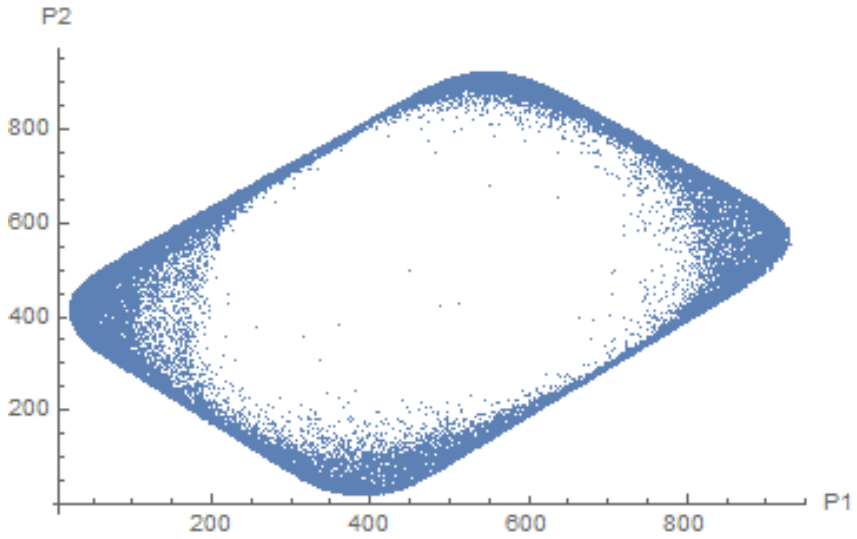

Figure 3: A squircle

Phase Change at the Nanoscale

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The basis of nanotechnology is the nanoparticle (NP), a unit of matter with a critical diameter between 1 and 100nm. Nanoparticles are currently used in a diverse range of applications, including: medicine (as synthetic skin, antioxidants, targeted delivery of drugs); manufacturing (flexible screens, packaging, fabrics); environment (breaking down oil, catalysts); energy (in fuel cells, batteries, solar cells) etc. In many of these applications the particles are exposed to high temperatures and so it is important to understand their response to a harsh thermal environment.

The theory of phase change at the macroscale is well established, however, as the length-scale decreases the physical process starts to exhibit unusual behaviour. One reason for the change in behaviour is that nanoparticles have a very large ratio of surface to volume atoms and so surface properties rather than bulk properties dominate. This results in a mathematical description that differs significantly from that at the macroscale.

In this talk we will discuss various issues that arise when modelling phase change at the nanoscale:

1. We present a novel formulation for the Stefan problem that reflects the fact material properties, such as latent heat and melt temperature, are size dependent.

2. A standard simplification is to study the one-phase problem, where one of the phases is set to the phase change temperature. When the phase change temperature varies this formulation loses energy.

3. Experiments at the nanoscale demonstrate that the well-known heat equation, based on Fourier's law no longer holds. More complex models, which exhibit heat waves must then be considered.

4. Finally, we show that the Stefan problem is analogous to that governing nanocrystal growth from solution.

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Thermal Transport Equations and Boundary Conditions at the Nanoscale

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Advances in manufacturing processes have brought us to the stage where reliable nanoscale devices are now commonplace. However, in most current and predicted applications of nanostructures, there is a strong concern over the management of heat [1]. The ability to successfully manipulate heat can be vital to device performance and a lack of thermal regulation can lead to melting and device failure [2]. In addition, experiments have shown that at sufficiently short length or time-scales Fourier's law breaks down [3].

The Guyer–Krumhansl (GK) equation is an extension to the classical Fourier law that is particularly appealing from a theoretical point of view because it provides a link between kinetic and continuum models and is based on well-defined physical parameters. Moreover, the striking similarity between the GK and Navier–Stokes equations enables nanoscale heat transport to be conceptualised in terms of fluid mechanics, consequently allowing a transfer of idea and methods between the fields.

In this talk we will show how, subjected to a specific boundary condition analogous to the slip conditions for fluids, the GK equation yields promising results in predicting the effective thermal conductivity of nanowires with circular and rectangular cross-sections [4].

Acknowledgments Marc Calvo-Schwarzwälder acknowledges the financial support of the 'La Caixa' Foundation.

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Mathematical Modelling of Nanocrystal Growth

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It is well-known that many properties of nanoparticles, such as luminescence, photostability, optical radiation efficiencies and electric properties among others, are size dependent [1]. Hence, the ability to create nanoparticles of a specific size is crucial. Using the precipitation method, monodisperse spherical nanoparticles can be generated following the line of the classical La Mer and Dinegar synthesis strategy where nucleation and growth are separated [2]. Through kinetic control of the reaction conditions, innovative methods to synthesize nanoparticles have been developed [3, 4].

In this talk we will describe a model for the process of synthesizing nanoparticles of the required size from a liquid solution. Initially, we will consider a single particle model that accounts for monomer diffusion in solution around the particle and kinetic reactions at the particle surface. The model consists of a diffusion equation for the concentration of the solution and a mass balance (equivalent to a Stefan condition) for the evolving particle radius. For the far-field bulk concentration, a mass conservation expression is used. Based on a small dimensionless parameter, we propose a pseudo-steady state approximation to the model. The model is then extended to a system of N particles and numerical solutions for the time-dependent average particle radius and standard deviation compared to experimental data are shown.

Acknowledgments Claudia Fanelli acknowledges financial support from the Spanish Ministry of Economy and Competitiveness, through the "María de Maeztu" Programme for Units of Excellence in R&D (MDM-2014-0445).

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Modelling Coffee Extraction Using Two-Phase Flow Equations

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The extraction of soluble material from a porous bed of roast and ground coffee relies on several complex physical mechanisms. Thus, achieving a dilute coffee solution with the desired chemical composition is a challenging endeavour. The key controlling mechanisms depend on the raw coffee properties, the roasting and grinding conditions, the water chemistry and the extraction method. An understanding of the dominant behaviour is key to consistently achieving coffee brew with the desired characteristics.

In this work, we build on recently developed models of coffee extraction [1]. The assumptions of one-dimensional flow (cylindrical geometry) and a uniform inlet source are relaxed to consider the influence of geometry and flow behaviour on extraction uniformity. The system is modelled using two-phase flow equations with interphase mass transfer. Flow behaviour is analysed using computational fluid dynamics software (CFD). The extraction behaviour is strongly dependent on the coffee grind size distribution. Rapid initial extraction is driven by low mass transfer resistance in smaller grains and the broken surfaces of larger grains. Slower extraction from the intact kernels of larger grains, limited by a higher mass transfer resistance, sustains extraction in the later stages of brewing. Numerical solutions are compared to analytic solutions of simplified systems. Extraction behaviour is compared to available experimental data.

Acknowledgments The authors would like to acknowledge funding under Science Foundation Ireland grant "Modelling of Multi-Phase Transport Processes to Enable Automation in Manufacturing, (MOMEnTUM)" – (14/SP/2750) and under the Dairy Processing Technology Centre (DPTC), supported by Enterprise Ireland grant agreement number TC 2014 0016. This work was also supported by 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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Asymptotic Analysis of the Guyer-Krumhansl-Stefan Model for Nanoscale Solidification

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Finely controlled ultra-fast solidification processes that give rise to nanoscale solids are becoming increasingly relevant in nanodevice fabrication. However, thermal transport on the nanoscale is not well described by Fourier's law, limiting the predictive capability of the classical Stefan problem. In this talk, the impact of non-Fourier heat conduction on nanoscale solidification is studied by coupling the Stefan condition to the Guyer–Krumhansl (GK) equation. The GK equation is an extension of Fourier's law, valid at the nanoscale, that is non-local in time and space. A systematic asymptotic analysis reveals that the solidification process can be decomposed into multiple time regimes, each characterised by a non-classical mode of thermal transport and unique solidification kinetics. For sufficiently large times, Fourier's law is recovered. The model is able to capture the change in the effective thermal conductivity of the solid during its growth, consistent with experimental observations. The results from this study provide key quantitative insights that can be used to control rapid nanoscale solidification processes.

Acknowledgments This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 707658.

Production Schedule Optimization by Applying Stochastic Network Programming

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Numerous manufacturing companies aim at designing their business processes as efficiently as possible to keep their position in the market. Making thoughtful decisions implies well-prepared planning. With the use of operations management network methods, for instance relocation or generalized network model, production processes can be easily and effectively modelled and optimized [1][2]. One of the most important task is to identify those activities within a process, which has the biggest impact on the process lead time. CPM and MPM are widely applied to this purpose [3]. Furthermore, regarding the operations in reality, processes are executed different times. Therefore, uncertainty and stochastic elements must be included in the model [4].

In our research a wooden box manufacturing enterprise was examined. In order to determine the features of the process 50 measurements were performed for each activity. These data were the basis in the determination of the process's probability distributions. Total lead time, critital path, time slacks were calculated with the use of CPM. On the basis of the results, Monte-Carlo simulation was applied, with which the critical path of the process were identified and time slacks were analysed and evaluated with the use of simulation. The reason for using this method over widely applied PERT method is that PERT assumes beta distribution which is not always proper. In addition, activity times were stochastic, so the critical path can change, which can mislead the dicision maker. As it was expected, the process' critical path changed many times, and time slacks significantly altered as well. Therefore, it is advisable to apply compute-intensive Monte-Carlo simulation, and in return, decision makers can make well-considered plan.

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Mathematical Modelling of the Hydration Process in Contact Lens Production

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In this talk we present a mathematical model of an industrially motivated problem, which arises in the production of soft contact lenses using a cast-moulding technique. The first step of the manufacturing process involves casting a liquid monomer along with an inert diluent between two moulds which define the shape of the lens. The polymerisation is initiated by curing under UV light, during which the monomer molecules react to form the polymer chains of the solid lens. The diluent is used in order to reduce the shrinkage of the lens during this stage, and is later replaced by water.

The hydration process follows, during which the diluent as well as any impurities or unreacted monomers are removed from the lenses. The hydration process is the rate limiting step on the production line, and optimising this stage is of particular interest to contact lens producers. This involves a detailed understanding of the physical processes at hand. We focus on modelling the removal of the chemical diluent (CD) in the process. This is removed by washing the lenses with an organic solvent (OS), which is subsequently removed by washing with deionised water. We model this CD removal using a coupled set of Partial Differential Equations, which describe volume fractions of both the CD and the OS.

The problem is posed as a one dimensional moving boundary problem, or Stefan problem, which is a particular type of boundary value problem in which the phase boundaries can move with time. In this problem we have two moving boundaries. The swelling lens increases with volume and this moving boundary is called the swelling front. There is also a moving boundary propagating inwards with the absorption of the OS which we call the diffusing front. Diffusion of CD within the swollen region is also modelled with the aim of understanding the dominant mechanisms of extraction during the hydration process. We solve the system numerically using a front tracking method, and also discuss some interesting asymptotic approaches as well as comparisons with experimental data.

Acknowledgments The authors are grateful for the support of MACSI funded by Science Foundation of Ireland Investigator Award 12/IA/1683. This work was also supported by Science Foundation of Ireland grant "Modelling of Multi-Phase Transport Processes to Enable Automation in Manufacturing, (MOMEnTUM)"-(14/SP/2750).

Modelling of Oscillation Mark Formation in Industrial Steel Casting

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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. 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.

A recent asymptotic model [1] for the formation of fold-type oscillation marks is analysed further by considering varying viscosity in the flux region. In order to formulate our model we refer to the work by Hill *et al.* [2] which is more amenable than numerical models. 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]. The effects of three key-components are considered, namely the heat transfer coefficient, thermal contact resistance and the flux-viscosity relationship.

Acknowledgments The authors are grateful for the support of the Irish Research Council grant no. GOIPG/2014/1147, Science Foundation Ireland grant no. 12/IA/1683 and MI-NET grant no. COST-STSM-TD1409-160216-070364-70364.

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Mathematical Modelling of Drying Dairy Powders Through Spray Drying Technologies

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Many methods for drying products exist, from freeze drying batches of product to continuous process using spray drying technology. Use of spray dryers is common in the dairy industry to ensure long shelf life of dairy products. Product is pumped through an atomiser into a chamber in parallel with a hot air flow stream. The liquid within the droplets evaporate and a dried product is returned from this process. Although the process seems simple, there are many difficulties and unknown phenomena occurring within the drying chamber. Use of Computational Fluid Dynamics (CFD) permits instantaneous and detailed flow phenomena and particle-flow interactions to be explicitly observed. When developing a drying model, a balance must be achieved between accuracy of the drying particle and the practicality with incorporation into CFD.

The work here focuses on the development of a droplet drying model to predict the instantaneous interaction of the droplet with airflow. The typical stages of wet droplet to dry particle are investigated and modelled for incorporation into CFD. An uneven temperature distribution within the drying particle occurs due to the thermal properties of the wet particle, where the Biot number can be greater than 0.1 [1]. This aspect is taken into account by modelling the temperature distribution within the particle core. Mass flow rate from the drying particle is considered by diffusion through a porous crust. Hence, properties of the particle can have a major influence on the drying rate and temperature distribution across the particle. Here we investigate these influences and assess why dairy products dry at different rates and what are considered the major factors in particle drying kinetics.

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Numerical Simulation of Tubular Components with Multi Channels Using Water-Assisted Injection Moulding

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The design of components in automobile or consumer products has become more complex with dimensional variations, curves, multi-branches and connections especially using metals which leads to a high production cost. Components made with plastics are the best solution in mass production because of lower part weight, high corrosive resistance and mainly cost effective.To address these challenges water-assisted injection molding (WAIM) can play a key role. Comparing with the traditional injection molding techniques, WAIM is the most sustainable injection molding technique able to produce high quality polymeric parts with complex geometries, raw material savings, also allowing the elimination of post processing work of molded polymeric parts. The main objective of this work is to optimize methods to produce hollow polymeric parts with several branches and complex geometries. We use a new finite volume approach to predict WAIM processing parameters. Such as, filling and packing time of melt, injection and packing pressure, flow rate and injection pressure profile, water injection delay time, water hold time, water pressure, melt temperature to optimize the ongoing experimental studies. With this numerical methodology, it was possible to investigate the influence of different inserts and overflow geometries and fluid direction, being these results a good guidance to experimental studies. Our numerical approach is validated by comparing with the results obtained in previous studies. This innovative work will influence the production of multi-branched and complex geometry hollow parts and guide on the optimization of WAIM experimental studies.

Acknowledgments This work is supported by the Fundačao para a Ciência e a Tecnologia (FCT) and Centro2020 through the Project references: UID/Multi/04044/2013; PAMI - ROTEIRO/0328/2013 (Nº 022158); MATIS (CENTRO-01-0145-FEDER-000014 - 3362); Programa-2020FEDER-08/SI/2015 – 3383 and 17684.

MS 23: EU-MATHS-IN: Success Stories of Mathematical Technologies in Societal Challenges and Industry

Exactcure: Personnalization of Your Medical Digital Twin

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Inappropriate medications kill more people than car accidents do! 3 times more, costing France 10 billion euros of health insurance / year. Why is it so complex? We are all different, we differently respond to drugs. ExactCure leverages a proprietary Artificial Intelligence in order to create personalized biomodels of drugs. In the framework of pharmacokinetics modelling, personalization means that kinetic parameters need to be estimated/adjusted from personnalized data. For that purpose we have begun to develop cutting-edge technologies that allow rigorous and smart integration of such personalized data in our proprietary calibration pipeline. The underlying mathematical techniques form the cornerstone of very challenging collaborations between ExactCure and Inria. In this talk we will give an overview about the kind of challenge we try to tackle and the scientific problems we seek to address through collaborative work.

Energy Optimal Cruise Control for Individual and Platoons of Heavy-Duty Trucks

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The presentation reports on the development of new mathematical methods for the online computation of energy optimal controls (acceleration, deceleration, choice of gears (!)) of heavy-duty trucks. Among the challenges are the non-linear mixed-integer nature of the optimal controls, resulting vanishing constraints, and achieving real-time feasibility on the on-board hardware by adaptive multi-level optimization methods. New methods meeting these challenges are presented, which form the basis of the Predictive Powertrain Control (PPC), which now is standard equipment in the Daimler Actros heavy-duty truck. An additional challenge in view of upcoming autonomous driving vehicles is the exploitation of potential drag reduction for energy savings in the joint optimal feedback operation of platoons of trucks. Numerical results will be presented indicating relevant additional savings (based on joint work with Ottmar Gehring (Daimler), Christian Kirches (TU Braunschweig), Darshan Balaganchi Muralidhara and Johannes Schloeder (both IWR, Heidelberg University).

EU-MATHS-IN Introduction, Opportunities for Its Nodes, and Major On-Going Initiatives

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In the last 2 decades, many reports have been written on the relation between mathematics and industry. Some 10 years ago the OECD, via its Global Science Forum, issued a report on "Mathematics in Industry" [1]. This was followed immediately by a Forward Look project funded by the European Science Foundation, which led to both a book of success stories [2] and a final report containing detailed recommendations [3]. Recommendation 2 from this report reads: "In order to overcome geographical and scientific fragmentation, academic institutions and industry must share and disseminate best practises across Europe and disciplines via networks and digital means." This recommendation has been followed up and led to the formation of EU-MATHS-IN at the end of 2013, and its mission statement is fully in line with this. Currently, EU-MATHS-IN has 18 national networks on board, and the exchange of best practies is proving to be extremely useful and vital for European mathematics and its relations to industry.

Recommendation 1 from the aforementioned FL report reads: "Policy makers and funding organisations should join their efforts to fund mathematics activities through a European Institute of Mathematics for Innovation." Many of the activities that are currently carried out are in line with this recommendation, although the main aim is to establish a European Technology Platform. To achieve this, 2 workshops were held in Amsterdam in 2017, where industry presented their views on the use of "MSO" (mathematical modelling, simulation and optimisation), as well as a workshop in the Lorentz Center in Leiden in December: "Future and emerging mathematical technologies for Europe". Especially at the latter meeting, additional actions were defined, such as writing a FET Open project proposal and influencing the upcoming FET Proactive open consultation.

In this presentation, we will give an overview of these developments in more detail, and discuss the actions indicated associated with setting up a European Technology Platform for MSO. At the time of the conference, more information should be available on some of the actions undertaken.

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Mathematically Enhanced Atomistic Simulation of Diffusion in Advanced Energy Materials

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The diffusion of matter at the nanoscale plays a major role in a wide range of industrial applications, including metal-ion batteries and polymeric membranes. For the vastly popular Li-ion batteries, solid electrolytes constitute a promising alternative against conventional liquid electrolytes, which are flammable and difficult to further miniaturize. In particular, garnet $Li_7La_3Zr_2O_{12}$ (LLZO) has attracted much attention due to its high conductivity and voltage stability. In order to enhance the mobility of Li atoms, Ga/Al cations have been selectively doped in Li sites; however, an atomistic understanding of how the presence of Ga/Al affects the structure, path topology and Li-ion dynamics is lacking. Similarly, a molecular description of transport and adsorption in polymeric membranes is crucial to improve the material performance in diverse technological processes such as the capture of contaminants from flue gases or the adsorptive storage of natural gas. Molecular dynamics (MD) simulations have been widely used to study intrinsic properties of materials. However, batteries and membranes are difficult to study with MD because it often fails to provide adequate sampling, making it difficult to accurately estimate equilibrium and transport properties. Here, we apply the Generalized Shadow Hybrid Monte Carlo (GSHMC) [1], an effective technique to enhance sampling in molecular simulations, to study (i) Li diffusion in LLZO solid electrolytes, and, (ii) adsorption and transport of gas through a polyimide-based BDPA membrane. For the battery system, we show how the GSHMC method combined with our in-house integrators can accelerate simulations of Li-ion migration in Ga/Al doped LLZO at different temperatures. For the membrane, we employ a combination of GSHMC with a Modified Adaptive Integration Approach (MAIA) [2] to study the adsorption, collective and self-diffusivity regimes of natural gas in BDPA membranes.

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Imbalance Determination for Wind Turbines

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In the growing field of clean energy extraction from wind the topic of rotor imbalances of wind turbines is of vital importance for the operation, safety and lifetime consumption of the turbines. Approximately 20% - 50% of the wind turbines have significant rotor imbalances. The vibrations induced by imbalances lead to damages of important components, high repair expenses, and reduced output. The state of the art to identify rotor imbalance is an expensive on-site procedure. The goal was to replace this procedure by a method that only uses the vibrations of the turbine during operation for the imbalance determination. By adding a suitable sensor in the nacelle and transfer the data via an existing data connection, the determination of the imbalances can be done off-site. To this end, a mathematical model of the turbine in the shape of an operator or matrix was constructed that maps the imbalance to the resulting vibrations. Thus the problem of reconstructing an unknown imbalance from measured vibration data forms an inverse ill-posed problem that requires regularization techniques for its stable solution. Over a course of several years, several methods have been developed, starting with the case that the vibration data are collected during an operation with constant rotational speed. Later aerodynamic imbalances were included and the situation of operation with variable speed was investigated. More sophisticated algorithms were developed for the latter cases. Whereas in the first case the underlying differential equation system can be reduced to an algebraic equation system, the variable speed situation was modelled via a system of integral equations. The system is evaluated and inverted by tensor products allowing the use of Kronecker products in the implementation. In cooperation with Bachmann Monitoring the algorithms were tested in wind parks and implemented in the Condition Monitoring System that the company developed and distributes.

Acknowledgments The authors are grateful for the support of the FFG Austria (grant 818098, and 841288).

Unsupervised Classification of Routes and Plates from the TRAP2017 Dataset

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The advances and widespread availability of automatic Number Plate Reading Systems (NPRS) allow the collection of large amounts of traffic data [1]. For law enforcement agencies, this raises the problem of finding convenient techniques and tools to analyze such data, in order to find meaningful traffic patterns and identify anomalous and criminal behaviors [2]. To involve private and public researchers in this difficult yet critical task, the Italian National Police (INP) organized TRAP 2017, the First European Conference on Traffic Mining Applied to Police Activities, and they made available a sample of anonymized data collected through automatic NPRS challenging the researchers to extract usable knowledge from this unique dataset. Here, we present our contribution to the conference, which earned us the Best Paper Award [3]. The paper describes the efforts, pitfalls, and successes of applying unsupervised classification techniques to analyze the Trap2017 dataset. Guided by the informative perspective on the nature of the dataset obtained through a set of specifically-written perl/bash scripts, we devised an automated clustering tool implemented in python upon openly-available scientific libraries. By applying our tool on the original raw data it is possible to infer a set of trending behaviors for vehicles travelling over a route, yielding an instrument to classify both routes and plates. Our results show that addressing the main goal of the Trap2017 initiative ("to identify itineraries that could imply a criminal intent") is feasible even in the presence of an unlabeled and noisy dataset, provided that the unique characteristics of the problem are carefully considered. Albeit several optimizations for the tool are still under investigation, we believe that it may already pave the way to further research on the extraction of high-level travelling behaviors from gates transit records.

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Decision Support Heuristic for Dairy Farms

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After having a smart phone based microsimulation tool for the optimal decision to be made on selling/keeping the ill cow (mastitis), we have started a new applied research project to improve the quality of the decision and the profitability as well by utilizing local data of the given dairy farm instead of national average values of the critical parameters such as chances to get the illness again, length of the dry and productive periods etc. We report on the preliminary efficiency improvement results.

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Constrained Clustering and Diagrams for the Consolidation of Farmland

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In many regions farmers cultivate a number of rather small (and discontiguous) lots that are distributed over a wider area. This results in a non-favorable cost-structure for the production. The classical form of land consolidation is typically too expensive, too time-consuming and too rigid. In fact, quite often, just a few years after a classical land consolidation was completed, the degree of fragmentation is close to what it was before. Therefore consolidation based on *voluntary lend-lease agreements* has been suggested as a legally simple, economically convincing and extremely flexible alternative. In the past, the practical relevance of this approach was severely limited by the mathematical complexity of finding good (let alone optimal) reassignments.

We developed a new mathematical clustering approach establishing a close relation between constrained clustering and diagrams. In spite of the complexity of the underlying task, the new model leads to practically very efficient tools which are now used in practice. The analysis of the mathematical structure of the model provides proof of its favorable properties (existence of feasible power diagrams) and allows the derivation of efficient approximation algorithms (based on the approximation of certain semi-norm level sets by polytopes) with a provably small worst-case error bound. Implementations of the algorithms together with additional customized tools particularly for in depth economic evaluation of the redistribution lead to successive land-lease actions in practice.

(The work presented in this talk is based on various joint publications of the authors including [1], [2], [3]. Some work was done in collaboration with additional colleagues including A. Alpers, A. Lyckegaard and H. Poulsen [4], S. Borgwardt [5], and F. Klemm [6].)

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M4SE@Home
Math for Smart Energy at Home

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In this talk, we present one of the Math-Enterprise interaction success stories at Cemosis called *Math for Smart Energy project at Home* (M4SE@Home) [1] in collaboration with J.B. Caillau at Université Bourgogne Franche-Comté at that time, now at Université Côte dAzur. Cemosis is a research platform of the Universit é de Strasbourg at the interface of mathematics, other disciplines, enterprises, and society. Cemosis is a node of the french MSO network [2]. A Master internship and a Ph.D. student were involved in this project and coached by two Professors.

With the multiplications of photovoltaic panels and the possibility to use household electricity production at home in Germany, new problems emerged. Massive energy rejection causes disturbances in the electrical network. Energy distributors now impose regulations on household energy profiles in the form of an energy roadmap (E-roadmap) prescription at critical hours subject to various constraints such as the amount of energy that could be rejected in the electric network. The E-roadmap is built using various sources of information such as the weather forecast or the energy stock exchange, and feeds an Energy Management Gateway (EMG) controlling the energy storage and usage of the batteries. From the household perspective, the objective is to optimize the production efficiency by minimizing energy wastes and possibly maximizing profits during the E-roadmap free schedule.

In this talk, we present the modeling of the system including the regulatory aspects as well as the design of the algorithm behind the EMG. We discuss a few scenarios based on synthetic E-roadmaps.

Acknowledgments This work was funded by the French Agency for Mathematics in In- teraction with Enterprises and Society (AMIES). The authors would like to thank Marion Spreng for the great work during her Master internship.

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modELTES: Model Based Engineering and Control of Latent Heat Thermal Energy Storages

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Energy efficiency and rational use of energy resources are important measures to meet the ambitious EU energy transition goals. Latent heat thermal energy storages (LHTES) expose a high potential for the optimization of complex thermal energy systems, in particular for optimal load shifting strategies and waste heat recovery and integration.

Within the project modELTES, dynamical models for shell and tube LHTES have been developed, experimentally validated, and implemented in standard software for flow-sheet simulation and control system design. Real-time capable, these models support storage manufacturers and engineering companies in design, integration and optimal control of thermal networks. A nonlinear model-based observer has been designed and successfully tested on real process data. It robustly tracks storage-internal temperature fields and accurately predicts stored energy and the state of charge.

Industrial-grade phase change materials (PCM) for usage in LHTES often show non-ideal melting and solidification phenomena. In modELTES, three classes of phase transition models have been developed. They can be directly integrated into storage models to reproduce experimentally observed phenomena, such as hysteresis in the phase transition due to supercooling and solidification kinetics.

Storage performance critically depends on the thermal capacity of its PCM. Identification of potential PCM for a specific application and the subsequent calibration of phase transition models rely on exact thermophysical material data. Differential scanning calorimetry (DSC) is widely used adopting linear temperature ramps. Being a differential technique, DSC signals for low heating/cooling rates show a poor signal-to-noise ratio, and their generation is time-consuming. For higher rates, they suffer from smearing, rendering an exact localization of the phase change temperature range and peak impossible. A data-driven de-smearing method based on extrapolation to a hypothetical zero-heating-rate was developed and successfully applied to calibrate the hysteresis submodel for PCM. Furthermore, a dynamical model for the simulation of heat flows within a heat-flux DSC has been developed and tested. It is capable to lower the variation of melting peak and end temperatures by approx. 80% compared to the methodology described in the respective ISO norm, and thus to significantly reduce the experimental efforts.

Finally, a case study for the optimal design and integration of a LHTES in an industrial waste heat recovery system with Organic Rankine Cycle will be presented.

Acknowledgments All authors acknowledge support by the Austrian Research Promotion Agency within the BRIDGE project modELTES. A.S. also acknowledges support by the German Federal Ministry of Education and Research within the project MOPhaPro.

Numerical Simulation of Fluid Flow and Heat Transfer at a Blast Furnace Runner

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One of the major methods used by steelmaking industry is the basic oxygen steelmaking, which uses hot metal as feed material for steel production. It is obtained in the blast furnace (BF) alongside with slag, where both materials behave as fluids due to the high operation temperatures. Their removal takes place through a drilled opening in the side of the BF and the resulting jet of fluids falls over the blast furnace runner, a multi-layered concrete refractory structure designed to enable separation of both materials as they flow downstream.

In the framework of the Horizon 2020 societal challenge *Climate action, environment, resource efficiency and raw materials*, it is of interest to minimize the wear of the BF runner, which usually needs to have its first layer completely replaced after two months of usage. This wear is believed to be strongly related to the position of the critical isotherms and also to erosion due to both the impact of the jet of fluids and to their flow along the runner. The nature of the problem, with extreme heat posing a big challenge to experimentation, motivates the usage of numerical simulation in order to find these isotherms.

A problem-decoupling strategy was used to obtain the numerical solution of a three-dimensional thermo-hydrodynamic model based on a BF runner at the ArcelorMittal company in Veriña, Spain. The fluid phases –hot metal, slag and air– are assumed to be incompressible, with constant properties and the free surfaces separating them are found using the VOF method. The S2S model is used in order to account for thermal radiation.

The proposed methodology has been shown to be useful in order to predict the position of the critical isotherms as well as to further understand how fluid flow and heat transfer take place at BF runner. The computed temperatures are validated using experimental measures supplied by ArcelorMittal.

Acknowledgments This work was partially supported by FEDER and Xunta de Galicia funds under the ED431C 2017/60 grant, by the Ministry of Economy, Industry and Competitiveness through the Plan Nacional de I+D+i (MTM2015-68275-R) and the grant BES-2016-077228.

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Advanced Computational Modelling in the Design of New Cardiac Radiofrequency Ablation Strategies

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Ablative techniques based on radiofrequency energy are used to produce localized heating of targeted biological tissue. In recent years there has been rapid growth in the number of new medical procedures employing these techniques, accompanied by the emergence of new electrode designs and energy delivery protocols.

In particular, radiofrequency ablation (RFA) is a common procedure in cardiac catheterization for the treatment of arrhythmias. Although globally a pretty safe procedure, it may present some risk. Thrombus formation can occur during RFA at the electrode-tissue interface when the temperature exceeds 80°C. Open-irrigated electrodes have been developed to reduce the risk of thrombus formation by cooling the electrode-tissue interface, allowing higher RF power delivery and the creation of larger lesions. On the other hand, higher RF power delivery increases the risk of steam pops occurrence, rather serious complication. Steam pops are caused by tissue overheating above 99°C, and may trigger explosive ruptures of myocardium. If the steam pop occurs sufficiently deep in the tissue, or if the RFA procedure is performed on atria, whose walls are thinner than the ones of the ventricles, such explosive rupture may result in a perforation of the cardiac chamber wall, and in dramatic hemorrhagic events.

We will discuss the role of advanced computational modelling in designing safer and more efficient ablation strategies to be applied in the clinical environment, and present the results we obtained in collaboration with the hospital de la Santa Creu i San Pau in Barcelona, as well as some biomedical company.

Acknowledgments The authors are grateful for the support of the Basque Government through the BERC 2014-2017 program and of the Spanish Ministry of Economy and Competitiveness MINECO through the BCAM Severo Ochoa excellence accreditation SEV-2013-0323, and Grant MTM2015-69992-R form the "Plan Estatal de Investigación, Desarrollo e Innovación Orientada a los Retos de la Sociedad" .

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Novel Modelling, Simulation, and Optimisation Paradigms in a Data Rich Environment

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Most companies are facing today an accelerated innovation dynamics and must address rapid changes of their respective environments. At the same time, digitizing opens new perspectives. Exploitation data, combined to the power of models used to design current products, enable unprecedented optimizations, anticipated maintenance and new services to the customers. Europe possesses historical assets in the field, relying on its expertise and the worldwide positioning of its simulation firms. The developments resulting from this vision offer ground-breaking opportunities for Europe in terms of economic and scientific opportunities.

Our industry team has gathered from the national counterparts of EU-MATHS-IN, established as a result of the ESF Forward Look report on "Mathematics and Industry" [1]. Within the last months we have worked on a white paper highlighting economical and technological opportunities and corresponding research needs. The specificity of the suggested approach relies on new model-based paradigms along the lines of the digital twin vision [2], in complementarity with High Performance Computing and Data Analysis initiatives.

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Accelerated Finite Element Simulation of Induction Machines

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Under the current social concern on sustainable energy consumption, the design of efficient electrical machines is an important challenge to be faced. In this framework, developing fast and accurate numerical methods plays a crucial role in the design and analysis of these devices. Indeed, the use of numerical tools prevents the building of unnecessary prototypes and significantly reduces both cost and time to obtain new configurations, while ensuring their rentability. A popular technique for this purpose consists in approximating, by means of a finite element method, the solution to a non-linear transient eddy current problem, eventually coupled with thermal, mechanical and/or electric circuit equations (see [2] and references therein).

The objective of this contribution is to present a novel and efficient methodology to reduce the time needed to reach the steady-state in the simulation of induction machines with squirrel cage rotor (see [1]), developed under a contract established between Robert Bosch GmbH and ITMATI. The technique is meant as a pre-computation for motor-oriented simulation tools that solve the electromagnetic problem describing the behaviour of the induction motor. Specifically, it is based on approximating suitable initial currents in the rotor bars of the squirrel cage, in such a way that the steady-state solution is achieved in only a few number of cycles. This method could represent a great advantage in terms of competitiveness because, since the initial currents are typically assumed to be zero, these kind of simulations usually take a very large CPU time.

In the presentation, we will address the problem motivation, describe the mathematical tools developed for its solution and show some numerical results to illustrate the applicability of the proposed methodology. In particular, the method will be applied to a particular induction machine working under different operating points. The results show important computational savings to reach the steady-state operation of the motor in comparison with assuming null initial conditions, what validates the efficiency of the procedure.

Acknowledgments The authors express their gratitude to Dr Marcus Alexander and Dr Stefan Kurz from Robert Bosch GmbH for useful discussions about induction machines and for providing them the data for the numerical experiments.

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Running H2020 projects of EU-MATHS-IN: MSO4SC and ROMSOC

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This talk will show two major ongoing initiatives, promoted by the European Services Network of Mathematics for Industry and Innovation (EU-MATHS-IN), in the framework of the H2020 Program:

1. **MSO4SC (Mathematical Modelling, Simulation and Optimization for Societal Challenges with Scientific Computing)** is a running H2020-EINFRA project. Its main goal is to develop a HPC oriented cloud infrastructure that provides MSO software and their applications as service. This infrastructure hosts the open-source FEM and FVM based mathematical developing frameworks Feel++, FEniCS-HPC and OPM. Further, it provides advanced mathematical services for solving societal challenges in the areas of brain research, high fidelity magnets, porous media flows, floating wind turbine, urban air quality prediction and drug design. The main advantage of using the MSO4SC infrastructure is that it supports one-click deployment of its software to HPC machines and thus prevents users from tedious installation procedures. Moreover, it provides the ensemble running of simulations assisting optimization procedures. In the talk we present the MSO4SC infrastructure with its services and information on cooperation with the MSO4SC consortium (e.g. by providing mathematical software as service from its infrastructure).
2. **ROMSOC (Reduced Order Modelling, Simulation and Optimization of coupled System).** This project is framed within the Marie Sklodoska-Curie action, under the topic "H2020-MSCA-ITN-2017 Innovative Training Networks" and in a specific type of action for European Industrial Doctorates (EID). The ROM- SOC project has as its main objective to train, through an international network of research centers and companies, a new generation of creative and innovative researchers, capable of transforming knowledge and ideas in products and services. The EIDs are networks composed of at least two partners, one from academic and the other from industrial sector, established in two different countries of the European Union, through which an Early Stage Researcher (ESR) is hired, who must belong to a third country different from the previous ones. The selected researcher will be enrolled in a doctoral program and will be supervised jointly by the com- pany and the research organization. Each recruited researcher must spend 50% of their time in the company and another 50% in the research organization. ROMSOC project involves fifteen European research centers and eleven industrial partners. In the talk we present the main features of this interesting initiative.

Acknowledgments The authors are grateful for the support of the Horizon 2020 Re-search and Innovation Programme of the European Union (Grant agreements No 731063 and 7653746).

Understanding the Charging Problem in Scanning Electron Microscopy, Particle Detectors and E-Beam Lithography

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Scanning Electron Microscope (SEM) is the primary tool for investigating micro- and nanometer size objects. Usually the sample is coated with a thing film of gold or other conducting material. However, in many applications involving insulators, coating is either not possible or not desirable and SEM images become distorted and difficult to interpret due to sample charging. Similar problems are encountered in solid-state particle detectors and e-beam lithography. Mathematical modeling of this charging process is essential for choosing an optimal imaging regime and designing new SEM's.

Almost universally interaction between electron beams and insulating targets is modeled with semi-classical Monte-Carlo (MC) methods, where the trajectories of many individual particles subject to various scattering processes are traced in time in an attempt to estimate the resulting charge distributions and the secondary electron yield. Since available models tend to become computationally expensive, unreliable, and difficult to interpret, especially, at lower electron energies, a SEM producer (FEI Company) has posed a problem of either accelerating the existing codes or finding a better solution.

As a faster alternative to discrete MC simulations we have developed a finite-element code implementing a continuous approach to this problem via a coupled system of Drift-Diffusion-Reaction equations [1]. To make reliable predictions the code was calibrated against experimental data [2]. Our continuous approach is now gaining popularity in other applications, such as e-beam lithography.

Acknowledgments The authors are grateful to Thermo Fisher Scientific (formerly FEI) for their partial financial support.

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Adaptive Direct FEM Simulation of Turbulent Flow in FEniCS-HPC in the MSO4SC Web Portal

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The Fenics-HPC framework (http://www.fenics-hpc.org/) is represented at the MSO4SC (Mathematical Modelling, Simulation and Optimization for Societal Challenges with Sci- entific Computing - http://mso4sc.elmerex.hu/) project on both mathematical framework and pilot application levels.

In this talk we will present our work for mathematical modeling of the problems relevant to societal challenges such as:

- flow past an aircraft simulation to optimize drag and lift and reduce the fuel con- sumption,
- simulation of a floating wind turbine in the pursuit of obtaining clean energy
- using the this mathematical framework to teach a Massive Open On line Course (MOOC) to demonstrate the high performance computing concepts to the students where we can provide the necessary super-computing resources encapsulated as a cloud service.

Ground-Based Augmentation System Research at Indra Navia AS

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Since the beginning of the air-travelling era men needed to find a way to complete safe landings. The most common way of doing so was to navigate with visual aid unsupported by any automated system. With time the interest in travelling by air has grown and therefore the traffic at airports and during an approach became heavier. The need for automation was obvious, therefore the first landing systems were developed starting with a natural choice of bistatic radar based system. During the years to come the system has morphed into Instrument Landing System (ILS) and became standard and the only system allowed to serve for category III automated landings.

The appearance of GNSS systems has given a chance to use an alternative way of navigating planes during an approach, landing, departure and surface operations, however in the early days the idea was not easily adopted due to slow acceptance of modern technology and airline reluctance to invest.

Nowadays ILS is still an operational system but it is Ground-Based Augmentation System (GBAS) that is going to be a choice for new airports. The advantages of the system is operating on a single frequency for the entire airport whereas ILS requires a separate frequency for each runway end. Usually the architecture of GBAS requires installation of four antennas and centralised building with four receivers and analyzer. Based on differences between received GNSS location information and a previously surveyed one the system obtains nominal error in location estimates. This error serves as base information for approaching aircraft on its approximate location and possible deviation from it.

The performance of the GBAS system relies on the quality of received GNSS signal which can be weakened or deformed by tropospheric and ionospheric conditions, Radio Frequency Interference (RFI), ephemeris error, multipath and more. Addressing and controlling these possible interferences brings GBAS to the top of currently used precision approach solutions.

Currently, focusing on RFI effects is a main topic of my research at Indra Navia AS.

MS 24: Modern Stochastic Valuation Techniques in Insurance

Pricing and Hedging Long-Dated Options and Guarantees

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The management of financial risks in insurance products calls for state-of-the-art models and modern calculation techniques. We will discuss some of the underlying models and hedging strategies for managing market risks under Solvency 2 and IFRS 4 Phase 2. Though technically very convenient, the assumption of deterministic volatility and interest rates does not find its justification in the financial markets for equity, FX or inflation-linked products [1][2]. In particular for long-dated insurance products, it is of importance that stochastic volatility and stochastic interest rates are jointly taken into account for a realistic modelling of the underlying risks. In this presentation we will give an overview of available stochastic methods which are useful for the pricing and hedging of long-term products with guarantees. Furthermore, to make these techniques applicable in practice, efficient models and simulation techniques are a must [3]; to this end, we will demonstrate that using GPUs (graphic cards) extreme performance boosts can be realized over traditional cashflow systems, facilitating advanced performance attributions and risk management practices. As a practical example we will look at the pricing and hedging of a large variable book, and compare different models and their computational performance.

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Stochastic Mortality Models

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As from 1/1/2016 all European based insurance and reinsurance companies have to comply with the so-called Solvency 2 regime [1]. Solvency 2 contains a new set of rules and requirements that are based on market valuation of the assets and liabilities and are meant to stipulate required capital in line with the real underlying economic risks. For the insurance sector such important component is mortality risk (the risk of people dying earlier for mortality and the risk of policyholders living longer for longevity). Although Solvency 2 prescribes a standard method for calculating required capital for mortality risk. This standard method assume a single, across-the-board factor for calculating mortality charge. Companies are allowed to deviate from that if and when their experience and portfolio composition supports. Therefore it is of importance to companies that they are able to construct and assess the loss distribution of mortality exposures for their own portfolio. In this presentation therefore we will give an overview of available stochastic methods that may come handy when facing this problem [2]. We will describe a few simple models, their advantages and disadvantages and available goodness-of-fit tests for comparing them. As a practical example we will use Hungarian population mortality data to compare different models.

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Stochastic Models in Claims Reserving on Actual Data

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Insurance and reinsurance institutions, particularly property and casualty insurers, put a considerable amount of effort into the understanding of outstanding claims reserves. Recently, increasing computational power has resulted in the development of more advanced claims reserving techniques, allowing the stochastic branch to overcome deterministic methods, which resulted in forecasts of enhanced quality. Hence, not only point estimates, but predictive distributions can also be generated in order to forecast future claim amounts. The significant expansion in the variety of models has not been accompanied by a comparable enthusiasm to validate these methods and to create supporting techniques for appropriate decision making. Papers [1] and [2] address the theoretical problem.

New models are introduced in [3], using not only the individual insurers', but collective claims observations from other companies for calibration. Among others, they apply experience ratemaking embedded into the credibility bootstrap overdispersed Poisson model. Authorities collect vast amount of information from insurance companies, and the question is whether or not these data can improve individual approximations. The purpose is to (1) get acquainted with the reserving methods and (2) present the decision making in model selection, supported by calculating goodness-of-fit measures of the actual and predictive distributions. Data stem from real observations from the National Association of Insurance Commissioners (NAIC). Measures used are probability integral transform, continuously ranked probability score, coverage and sharpness.

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Risk-Free Curves in Stochastic Environment

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Interest rate curves are essential objects of modelling for insurance companies, as most of the guarantees they are selling have a strong dependency on the term structure of interest rates. In order to arrive from a finite number of market observations to a full interest rate term structure that is defined for any positive maturity, one has to handle three problems that might require a methodology on its own: bootstrapping, interpolation, and extrapolation. For valuation of insurance liabilities this risk-free curve methodology is prescribed by the regulator EIOPA [1], and is based on the Smith-Wilson method [2]. Tackling all three problems at once is one of the big advantages of this method. A disadvantage is that it involves a computationally intensive optimization problem, causing the curve calculation a hot spot in a risk calculation engine, when the curves are subject to Monte-Carlo sampling. In the presentation we will show how the calculation of these risk-free curves can be sped-up by means of a neural network using Keras [3] frontend of TensorFlow [4].

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MS 25: Optimization Success Stories with Portuguese Industry

Designing a Logistics System Using a Location-Routing Approach

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In the location analysis literature, location-routing concerns approaches that simultaneously address location and routing decisions [1]. These integrated approaches may lead to more efficient overall solutions than when addressing location and routing separately [2]. This has motivated the application of such approaches in several real-world scenarios, which can be found in logistics, telecommunications, road maintenance, etc. [1, 3].

This talk addresses the design of a logistics system, in the region of Lisbon, for a company distributing products with uncertainty regarding demand quantity and locations. To tackle this challenge, a location-routing model was used, supporting a newly proposed methodology for the company's distribution. Results for this new approach will be presented and discussed.

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The Role of Optimization on Multi-Material 3D Printing Using Stereolithography

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Three-dimensional printing, or 3D printing, is an additive process for rapid free form manufacturing, where the final component is created by the addition of successive layers of material. Each layer is a cross-section of the new component, thus the printer draws it as in 2D. Several improvements have been made to 3D printing methods ever since their origin and nowadays this type of printers has become fairly popular.

One of the main goals of the project "NEXT.Parts" is to design, and build, a 3D printer that is able to produce components with more than one material. The new technique aims to respond to the demand for reliable and costly to produce complex parts in small series that combine several materials, with a wide range of applications, whenever overmolding is not viable. Despite their potential, 3D printers capable of working with more than one materials are yet unknown.

The new apparatus uses stereolithography, where a laser polymerizes part of a liquid polymer, one thin layer at a time. Additionally, it prints components in which the polymer covers a previously constructed 3D grid structure of a different material. The existence of a given grid that supports the polymer brings additional difficulties, resulting from the possible "shaded" areas on the surface of the polymer. This issue is addressed by installing additional light emitters on the walls of the printer, which raises two questions:

1. What is the least number of emitters to use, so that all the cells of the component are polymerized, and where should they be installed?

2. How to assign the cells to polymerize and the emitters?

It will be shown that the answer to the first question can be given by means of combinatorial optimization, namely by solving a set covering formulation. The second problem will be formulated as a linear integer problem with both covering and assignment constraints. This formulation takes into account the quality of the printed component (related with the distortion of the light over the printing surface) as well as the number emitters activated for each layer. Algorithmic methods for the two problems will be described and discussed.

Acknowledgments This work is co-financed by project PT2020-POCI-SII & DT 17963: NEXT.Parts, Next-Generation of Advanced Hybrid Parts. MP is partially supported by CMUC - UID/MAT/00324/2013, funded by the Portuguese Government through FCT/MEC and by the European Regional Development Fund through the Partnership Agreement PT2020.

Reverse Logistics Modelling of Assets Acquisition in a Liquefied Propane Gas Company

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This work addresses an industrial challenge that consisted in planning the acquisition of liquefied petroleum gas (LPG) cylinders. The challenge was proposed at an European Study Group with Industry, by a Portuguese company that started its activity in the production and distribution of biofuel and, since then, has extended its business areas to other fuels and energy. The objective was to define an assets acquisition plan, i.e., to determine the amount of LPG cylinders to acquire, and when to acquire them, in order to optimize the investment.

Classical inventory models, such as the Wilson model, determine the Economic Order Quantity (EOQ) as the batch size that minimizes the total cost of stock management. A drawback of this approach is that it does not take into account reverse logistics, which in this challenge (i.e. the return of cylinders) plays a crucial role. Richter [2] extended the EOQ model to allow the incorporation of used products, which were repaired and incorporated in production. It assumes a stationary demand in a model with two shops, where the first shop is producing new products and repairing products used by the second shop. Also considering deterministic demand and reverse logistics is the model proposed by Teunter [3], differing in allowing to consider varying disposal rates and disaggregating holding costs. Other developments on the EOQ model are by Alivoni *et al.* [1]. They propose a stochastic model where production or purchase of new items integrates product reuse, in order to identify the need of placing a production/purchasing order to avoid stock-out situations.

By forecasting the demand, sales and return of LPG cylinders, it is possible to use them as the input values of demand and return rate, applying to the data the inventory models with reverse flows.

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On the Scheduling of Periodic Events

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How should N regular polygons be inscribed on a circle so that the minimum distance between two adjacent vertices is as large as possible? How should trains that arrive at a railway station in constant intervals a_i be scheduled so that the safety interval between two trains is maximum? These are different specifications of the same problem: Given a collection A of N (possible repeated) positive integers a_i, find $\delta_i \geq 0$, for $i = 1, \ldots, N$, such that $z = \min |m\, a_i + \delta_i - (n\, a_j + \delta_j)|$, for $i, j = 1, \ldots, N, i \neq j$ and $m, n \in \mathbb{N}_0$ is maximum.

The problem has been addressed by Burkard [1], who solved the problem for $N = 2$ and for arbitrary N but with no more than two distinct values in A, and latter by Vince [2]. Using graphs Vince [2] solved the problem for $N = 3$, showed the problem can be solved by a finite search by defining a finite set of rational numbers that includes an optimal solution, and proved the problem is NP-hard.

Here we present Mixed Integer Linear Programming (MILP) formulations for the problem, describe a procedure to obtain bounds on maximum z, and report computational results. We also consider the restricted version where for every pair $i, j = 1, \ldots, N, i \neq j$, $|\delta_j - \delta_i| \leq \gcd(a_i, a_j)$, the greatest common divisor of a_i and a_j. For the restricted version we give a combinatorial procedure that finds optimal solutions, compare the performance of this approach with the MILP model, and prove that the problem is NP-hard.

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MS 26: ECMI Special Interest Group: Maths for the Digital Factory

Optimal Inflow Control in Supply Systems with Uncertain Demands

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We are concerned with optimal control strategies subject to uncertain demands. They have a broad range of applications. Taking uncertainty into account becomes more and more important in many areas. In the context of supply chain management, a need for control strategies taking these uncertainties into account naturally arises when it comes to production planning. Deviations from the demand actually realized need to be compensated, which might be very costly and should be avoided. To this end, we consider different approaches to control the produced amount at a given time to meet the stochastic demand in an optimal way. Supply chains are represented by transport equations and stochastic differential equations are used to model the uncertain demand. Finally, the approaches will be compared in a numerical simulation study.

Acknowledgments The authors are grateful for the support of the German Research Foundation (DFG) within the project "*Novel models and control for networked problems: from discrete event to continuous dynamics*" (GO1920/4-1).

Optimal Control for Hot Rolling of Multiphase Steels

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Multiphase steels combine good formability properties with high strength and have therefore become important construction materials, especially in automotive industry. The essential industrial process route for the production of multiphase steel consists of the hot rolling and subsequent controlled cooling to adjust the desired microstructure in steel, i.e., the composition of steel phases produced upon cooling. The most important control parameters are the flow-rate of water and the feed velocity of the strip. Since the process window for the adjustment of the phase composition is very tight, the computation of optimal process parameters is an important task.

The problem of the controlled cooling can be considered as an optimal control problem. The state equations are a semilinear heat equation coupled with an ordinary differential equation, that describes the evolution of the steel microstructure [1]. The time-dependent heat transfer coefficient serves as a control function [2]. Due to the nonlinearity, the state system requires a detailed analysis, especially concerning the regularity of the solutions, which is of crucial importance for the derivation of second-order sufficient optimality conditions.

For the numerical solution of the control problem reduced sequential quadratic programming method with a primal-dual active set strategy is applied. The numerical results are presented for the optimal control of a cooling line for production of hot rolled dual phase steel.

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Simulation and Optimization of Thermal Distortions for Milling Processes

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The material removal by a rotating milling tool generates mechanical oscillations of the machinery as well as local forces and heat flux acting on the workpiece. All of those lead to inexact material removal and can produce a bad quality of machined surfaces. We describe the modelling and simulation of such processes, involving systems of parabolic and hyperbolic/elliptic equations on time dependent domains. Based on these, we present approaches to control or optimize the results. Depending on the aspect under investigation, global macroscopic or local mesoscopic effects are modeled and simulated. Finite element methods with a subdomain approach can be used to discretize the problem. Numerical simulations and some optimization and compensation strategies and results will be presented, with some comparison between simulations and experimental data [1, 2].

This is partly joint work with Carsten Niebuhr and Jost Vehmeyer (both University of Bremen) as well as Daniel Niederwestberg and Berend Denkena (both IFW, University of Hannover) and Jonathan Montalvo-Urquizo and Maria Villarreal-Marroquin (both CIMAT Monterrey, Mexico).

Acknowledgments The authors are grateful for the support of DFG via SPP 1480 (grant MA 1657/21-3) and DAAD/CONACYT via PPP.

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Modeling and Simulation Approaches for the Production Functional Parts in Micro Scale

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In modern production engineering processes, miniaturization is of growing interest. Due to the challenges arising when transferring cold forming process from macro to micro range, such as size effects, the Collaborative Research Center "micro cold forming" was founded in 2007. Its central concern is the supply of methods and processes for a systematic design of reliable micro cold forming processes. The projects within the CRC focus not only on developing new forming methods for metallic micro components smaller than 1 mm, but also address their implementation in industrial applications in order to produce hundreds or thousands of pieces per minute.

In this talk, we consider the process chain for the production of functional parts using on an alternative cold forming process for rods that consists of an master forming step based on laser melting and an subsequent forming step. After briefly describing the process chain of this process and addressing some arising challenges, we will focus on modeling and simulation approaches for the laser based master forming step, which is crucial for the quality of the product.

The master forming step, producing a so-called *preform*, can be modeled with PDEs by coupling the Stefan problem with the incompressible Navier-Stokes equations where we have a capillary boundary condition for the melt. In regards to the simulation, a finite element method based on combining the enthalpy approach with an ALE method is used for a rotational symmetric process design when the heat source is coaxially applied to the work piece. Since a parameter study shows that the efficiency of this setup decreases significantly for long irradiation times, a new process design has been developed using a lateral applied laser heat source. This setup is also convenient to generate preforms at sheets or more complex geometries, however, as we no longer can reduce the model to a 2D rotational symmetric situation, a full 3D finite element simulation is needed to analyze the process. To find close to optimal process parameters, the concept "optimization-via-simulation" is used. This concept allows for finding suitable parameters while keeping the number of simulation runs to a minimum.

While this first simulation approach is based on a 3D enthalpy method with remeshing, a much more flexible simulation framework can be implemented by the use of the eXtended finite element method. Thereby, not only the work piece but also its surroundings can be considered with a model. This is especially important when heat dissipation mechanisms such as heat losses arising due tot the use of shielding gas have to be modeled. In an outlook, we present our work on the XFEM framework `miXFEM` which bases on the `FEniCS` project and makes use of automated code generation.

Acknowledgments The authors gratefully acknowledge the financial support by the DFG (German Research Foundation) for the subproject A3 within the Collaborative Research Center SFB 747 "Mikrokaltumformen - Prozesse, Charakterisierung, Optimierung".

MS 27: MSO for Steel Production and Manufacturing

Modeling and Optimization of a Gas-Stirred Liquid Flow for Steelmaking Processes

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Gas stirring is an important process used in the steelmaking industry to homogenize the temperature and the chemical composition of the liquid steel, and to remove inclusions which can be detrimental for the steel quality [1]. In this process, argon gas is injected from the bottom of the vessel through gas nozzles and rises by buoyancy through the liquid steel, thereby causing stirring, i.e., a mixing of the bath. The injected gas volumetric flow rate is the main process parameter in the industrial operations. This talk presents a mathematical model of the stirring, the results of numerical simulations and an optimization study to find out whether a constant or a sinusoidal stirring is better for the homogenization of the liquid steel. The model for the two-dimensional bath with a central gas nozzle is based on the work from Sahai and Guthrie [2]. The liquid flow is governed by the incompressible Navier–Stokes equations, while the effect of the gas is applied as a non-homogeneous Dirichlet boundary condition on the velocity of the vertical symmetry axis. A comparison of the simulation results with existing data from literature is performed to validate the model. In the optimization study, the bath homogenization is described by the vorticity field. The cost functional considers both the quantity and distribution of the vorticity in the liquid, while the boundary velocity represents the control variable. It is shown that, depending on the cost functional and initial conditions, the sinusoidal boundary velocity may lead to a slightly better distribution of vorticity. On the other hand, a constant and high boundary velocity contributes significantly to both quantity and distribution of vortices in the bath. In practice, this result suggests to operate stirring with a constant and maximum gas volumetric flow rate for a better homogenization of the liquid steel.

Acknowledgments The authors are grateful for the support of the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 675715 (MIMESIS).

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Modelling, Simulation and Optimization of Inductive Pre-Heating for Thermal Cutting of Steel Plates

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One of the final stages in the production of steel plates is the thermal cutting process. Flame cutting is a common and effective method for a wide range of thicknesses but can provoke undesired side-effects on the steel plates, such as cracks. The apparition of these anomalies depends on the material properties, the cutting parameters, the thickness of the plate and particularly on the temperature of the plate before cutting [1, 2]. A general practice to avoid cracks in high-strength steels consists in warming the plates uniformly just before cutting.

The aim of this work is to investigate local inductive pre-heating, which is a more energy-efficient strategy to uniform pre-heating of the plate. For this purpose, the simulation of flame cutting is required to understand the heat affected zone (HAZ)–the most sensible area for cracks. We use a quasi-stationary 3D-model similar to previous works from Thièbaud [3]. Once the HAZ has been identified, an optimal pre-heating can be added. This is performed by a thermoelectric 3D-model [4] which predicts the temperature distribution in the cutting line under the influence of an induction coil situated on top on the moving plate. Experimental data is used to validate both models that are employed to optimize the whole process. This project is in collaboration with steel-producing company SSAB.

Acknowledgments The authors are grateful for the support of the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No. 675715 (MIMESIS).

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Numerical Simulation of High-Frequency Induction Welding of Steel Tubes

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High-frequency induction (HFI) welding of tubes is a method of manufacturing welded steel tubes. First, a steel strip is formed into a tube shape. Subsequently, this is passed through an induction coil which heats the tube edges to welding temperature. The edges are then joined by mechanical pressure to form the welded tube. HFI welding is a multiphysics process which occurs in two stages: electromagnetic heating followed by mechanical joining of the tube edges. These can be mathematically formulated as partial differential equations. Finite element method(FEM) has been used to numerically discretize the HFIW process. The welding section is a part of a continuously moving production line. Hence, this process is modelled as a quasi-stationary process [1].
The electromagnetic heating is governed by Maxwell's equation in the time-harmonic regime and the classical heat equation. The three-dimensional computational mesh must resolve electrical skin depth which is much smaller than the tube dimensions. For this adaptive mesh refinement technique is used [2]. Electromagnetic and thermal material properties are non-linear with respect to temperature. The velocity of the tube incorporated in the convection term of thermal simulation is spatial function which is calculated for the tube. High welding line velocity requires stabilization of the numerical algorithm for the thermal simulation. The temperature profile of the tube edge is obtained from this electromagnetic heating simulation.
The mechanical joining of the tube edges is a large deformation problem with small strains. This is described by the material flow in a two-dimensional plate modelled by momentum balance. For the constitutive material model, viscoelastic behaviour of the steel is considered in the welding temperature range [3]. The temperature profile from the electromagnetic heating simulation results is then used to determine the temperature dependent mechanical properties of the tube edge. The shape of the weld joint as a result of the viscoelastic flow is also obtained.

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Induction Hardening of Cam Profiles: Modeling, Simulation, and Optimization

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Steel products frequently do not have the necessary properties to satisfy the application-specific demands in terms of wear resistance, strength and ductility. Heat treatment is therefore required to improve those features and increase the durability of the target piece. Induction hardening is a method for the surface heat treatment and holds a key role for steel parts coming from automotive and aerospace sector, such as gears, cams and shafts.[1]

In the case study presented a cam-like workpiece is considered for hardening with the aim of achieving a regular contour profile for temperature, which accounts for a regular hardening pattern as well. Numerical simulation provides a substantial advantage due to the possibility to tune the induction process parameters in order to achieve the desired results and avoiding a large number of empirical trials.

Based on a thermo-electromagnetic-metallurgical model for hardening [2], the development of a finite element simulation tool for the electromagnetic fields and induced currents, allows the numerical calculation of the time-variant temperature profile along the target part.

The shape of the inductor plays a pivotal role when generating and localizing eddy currents inside the workpiece and while the effect of input power and hardening time on the hardening profile is well understood in applications, it is the aim of this study, to investigate the influence of the inductor shape on the final hardening profile.

Acknowledgments The authors are grateful for the support from the European Union Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No. 675715.

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MS 28: Multidisciplinary Approaches to Biological Modelling

A Macroscopic Model of Riverine Microplastic Transport

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Microplastic is a piece of plastic with the size measured by the longest diameter ranging between 1 μm and 5 mm. Depending on the polymer substance, microplastic appears in aquatic environment in several forms including microfoam, microbead, microfibre, microfragment, and microfilm. There are many substances of microplastics particularly found in fresh water, but the most ubiquitous and abundant are polypropylene, polyethylene, and polystyrene. Under stagnant water, the internal density of microplastic determines its buoyancy – polyethylene and polystyrene are buoyant, while polypropylene can be both buoyant and retaining depending on the chemical composition. Rigorous studies on and data regarding how microplastics emit to fresh water are lacking, however processes such as industrial spillage of primary microplastics, deposition of household water containing skin care products and clothing–induced microfibres, regular washouts of automotive tyre particles on bridges, and long usage of ropes and brittle plastic materials in agriculture, have been postulated to be some pivotal sources of origin. As soon as microplastic enters into aquatic environment, it undergoes both adsorption and absorption of persistent organic materials (POPs) as well as desorption of the pollutants after biotal ingestion, therefore rendering particular toxicity and corsinogenicity to organic lives.

We develop a mathematical model for the transport of spatially distributed microplastics through a river with the flow field measured *a priori*. The fundamental idea behind the framework is that microplastics are considered as particles that move along the water flow. Each particle is considered to occupy a certain spatial location at a time instance with its particular size. The density of all particles with a certain space–time–size tuple follows a population balance equation (adopted from chemical reactor modeling framework) highlighting apparent physical properties: transient evolution, spatial transport, diffusion, breakage and sedimentation. Breakage indicates the process where a larger microplastic splits into smaller microplastics. Most plausible causes of breakage that are considered in the modeling are collisions among microplastics and between microplastics and solid materials (sand, waterfront buildings), weathering (UV exposure, overheating, high humidity), trophic transport and biofouling (biofilm formation on the surface) that pronounce embrittlement of the microplastics. Sedimentation is the process where particles settle at the bottom of the river or at some boundary. The rate of sedimentation in the model incorporates relevant causal phenomena including aggregation with organic materials and biofouling, low water velocity, sheer stress falling behind its particle–size–dependent critical values; and erosional phenomena including disaggregation and resuspension. Upon completion of model derivation, we determine the local existence and uniqueness of solution as well as its positivity and boundedness to certify non-blow-up dynamics. Proper numerical methods and possible coupling with the hydrodynamics are sought for further numerical investigation.

A Modified Hawk-Dove Game for Modelling Dominance, Sharing, and Learning

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Animals of the same species often find themselves in conflict over limited resources such as food, water, shelter, and mates. While it might be expected that this should lead to frequent fights, animals from sea anemones to primates have developed strategies for reducing or avoiding overt aggression when resolving disputes. One common strategy for avoiding extended fights is through the development of a stable dominance hierarchy; in many cases, this is characterised by an initial fighting phase followed by the submission of subordinates in all future encounters. Another possible strategy for avoiding extended fights is through the sharing of resources; the challenge of understanding sharing and other apparently altruistic actions has been of great interest (especially to theoreticians) over the last 40 years. However, reciprocal altruism appears to be significantly less common in social animals than dominance hierarchies.

In this talk, we present and discuss a simple mathematical model for exploring how asymmetries in fighting ability can destabilise sharing and promote the stability of a dominance relationship between two animals. Our model is based on an iterated version of the classical Hawk-Dove game, but modified so that one animal may have a greater chance of winning fights than its opponent. We analyse optimal strategies for the two animals when they are aware of the difference in their fighting ability, and extend this analysis to consider good strategies for the case where neither animal begins with any knowledge of its fighting ability or that of its opponent. We find that our results are qualitatively consistent with experimental observations; sharing is stable in certain parameter regimes, but in many cases the optimal strategies involve a period of fighting followed by the submission of a subordinate animal to a dominant animal.

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

Mathematical Modeling of the Heart Rate Variability

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From the pioneering work of Bernardi [1], it is known that the heart rate variability signal exhibits oscillation at the respiration frequency even at high workload exercise. Although it has been demonstrated in a non-continuous dynamic manner, the persistence of this phenomenon during continuously increasing exercise. Recently, we have introduced in [2] the time varying integral pulse frequency modulation model TVIPFM model that relates the observed amplitude of the mechanical modulation (MM) to the ventilation and the mean heart rate, with a set of subjects.

Our motivation is to analyze the heart rate variability (HRV) obtained by (TVIPFM) using time frequency representations. The estimated autonomic nervous system (ANS) is filtered around the respiration using a time varying filtering, during exercise stress testing. And after summing power of the filtered signal, we compare the power of the filtered modulation of the ANS obtained with smoothed pseudo Wigner-Ville representation, spectrogram and their reassignments. After, we use a student t-test ($p < 0.001$) to compare the power of HRV in the frequency band of respiration and elsewhere.

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Pattern Formation in a Homogenized Neural Field Model

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We study pattern formation in a homogenized 2-population nonlocal neural field model. The connectivity strengths are modelled by means of functions which are periodically modulated in both the synaptic footprints and the spatial scales. It is shown that the nonlocal synaptic interactions promote a finite band width instability, just as in the translational invariant case. The stability method which is a generalization of the method developed for the translational invariant case [1], relies on a sequence of wave-number dependent invariants of 2×2-matrices representing the sequence of Fourier-transformed linearized evolution equations for the perturbation imposed on the homogeneous background. The generic picture of the instability structure consists of a finite set of well-separated gain bands. We follow the instability into the nonlinear regime for both steep and shallow firing rate functions. In the weakly modulated regime the following picture emerges: For the steep firing rate functions stable spatial oscillations are formed whereas we get spatio-temporal oscillations in the shallow regime of the firing rate functions, consistent with the findings in the translational invariant case. In the regime beyond the weakly modulated case a rich plethora of phenomena takes place. The results reported here are based on [2].

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Design of Supercontinuum Optical Sources Aided by High Performance Computing

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Spectral white light is used in Optical Coherence Tomography (OCT) systems for e.g. medical diagnostics purposes. A powerful way of generating a broad band white light source is to use supercontinuum generation in nonlinear optical crystal fibers illuminated by a monochromatic laser. We discuss the development of a new generation of supercontinuum light sources with unprecedented low noise and shaped power spectra that are optimal for use in the next generation ultra-high resolution Optical Coherence Tomography (UHROCT) systems[1]. The overall goal is to use UHROCT for cost effective diagnose of glaucoma, the second leading cause of blindness worldwide, and to develop equipment easy to use for a local clinic contrary to current practice.

We invoke high performance computing of the generalized nonlinear Schrödinger equation for aiding the optimal design of supercontinuum generation. Our model includes higher order dispersion, delayed Raman response and tapering in order to optimize fiber design features for reducing the noise in a supercontinuum light source and shape its spectrum. The numerical model is based on state-of-the-art spectral methods implemented using modern parallel programming paradigms such as MPI and CUDA to run efficiently on contemporary and emerging parallel computing many-core hardware such as graphical processing units. Not only the hardware plays a role for fast computing, algorithm development is as important, and here we focus on the interaction picture method [2]. High performance computing has turned necessary in the study of super continuum generation mainly due to the complexity of the nonlinear wave (soliton) patterns requiring extremely high computational resolution. The project is conducted in collaboration with NKT Photonics, designing supercontinuum sources, and Bispebjerg Hospital, Denmark.

Acknowledgments The authors acknowledge financial support from Independent Research Fund Denmark (DFF) (LOISE—4184-00532B), Innovation Fund Denmark (SHAPEOCT—4107-00011B) and GALAHAD Horizon 2020 Framework Programme (H2020) (73 2613.)

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Dynamic Optimization and Game Theory Elucidate Vertical Migrations in the Ocean

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The dynamics of many biological and ecological systems are only partly determined by physical laws, but emerge also from the collective behavior and decisions of organisms in the system. A striking example of this is vertical migrations in the ocean; an ubiquitous phenomenon which has decisive effects on system-level properties, viz. the flow of energy through the food-web, and the flux of carbon from the atmosphere to the deep ocean. To understand and predict behavior of organisms, we may assume that this behaviour has been selected during evolution. If the organism is viewed in isolation, we anticipate that its behaviour solves an optimization problems, while multiple organisms should arrange themselves according to the equilibrium of a game. Here, I review recent work of myself and collaborators [1, 2], which poses dynamic optimization and game models of vertical behaviour of oceanic predators, specifically tuna, and the prey that constitute the Deep Scattering Layer. These models yield optimal behaviours that closely resemble actual observed behaviour and can therefore be utilized to predict behavioural responses to changing environments. I then present new results that exploit and clarify the connection between these optimization problems and classical mechanics. I finally discuss numerical methods for analyzing these models.

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Transitions from Trees to Cycles in Adaptive Biological Transport Networks

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Transport networks are crucial to the functioning of natural and technological systems. Nature features transport networks that are adaptive over a vast range of parameters, thus providing an impressive level of robustness in supply. Theoretical and experimental studies have found that real-world transport networks exhibit both tree-like motifs and cycles. When the network is subject to load fluctuations, the presence of cyclic motifs may help to reduce flow fluctuations and, thus, render supply in the network more robust. While previous studies considered network topology via optimization principles, here, we take a dynamical systems approach and study a simple model of a flow network with dynamically adapting weights (conductances). We assume a spatially non-uniform distribution of rapidly fluctuating loads in the sinks and investigate what network configurations are dynamically stable. The network converges to a spatially non-uniform stable configuration composed of both cyclic and tree-like structures. Cyclic structures emerge locally in a transcritical bifurcation as the amplitude of the load fluctuations is increased. The resulting adaptive dynamics thus partitions the network into two distinct regions with cyclic and tree-like structures. The location of the boundary between these two regions is determined by the amplitude of the fluctuations. These findings may explain why natural transport networks display cyclic structures in the micro-vascular regions near terminal nodes, but tree-like features in the regions with larger veins. [1].

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A New Model for the Inflammatory Stress Response

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There is current interest in coupling mechanisms between the acute inflammatory response and the Hypothalamic–Pituitary–Adrenal (HPA) axis, in mammals. The inflammatory response is activated acutely by pathogen- or damage-related molecular patterns, whereas the HPA axis maintains in the body a long-term level of the stress hormone cortisol, which is also anti-inflammatory.

A new integrated ODE model (ITIS model) of the interaction between these two subsystems of the inflammatory system is proposed. The ITIS model is capable of reproducing clinical data of tumor necrosis factor alpha, adrenocorticotropic hormone (ACTH) and cortisol, and suggests that repeated LPS injections lead to a deficient response. We describe here the construction of the system of differential equations, and discuss predictions resulting from the model.

MS 29: Finite-Sample System Identification

Data Perturbation Methods for Finite Sample Nonlinear Estimation and Uncertainty Quantification

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Estimation of unknown parameters in parametric models is a fundamental inference problem along with quantification of uncertainties for the obtained estimates. Complicating factors can be if the model is highly nonlinear, the sample size is small or there is little that can be assumed about the noise.

We present a randomized method that can provide guaranteed finite sample confidence regions for a very wide range of nonlinear estimation problems. The initial ideas for such a method were presented in [1] and [2], where a lot of room was left for choices that the user could make in terms of the *performance measure*. It is known that certain performance measures result in unwanted artifacts in the confidence regions, rendering them not always interpretable.

The main goal of the presentation is to offer insight into why performance measures of a specific type are more "natural" than others. Using these performance measures ensures a good level of interpretability for the resulting confidence regions.

We present a case study about tremor data from the Groningen gas fields. The setting is very appropriate as the data set contains ~ 100 data points, the connection between input and output is highly nonlinear and very little can be assumed about the external noise.

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Source Localization from Rss Measurements Using LSCR

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This contribution addresses the localization of an emitting source from noisy Received Signal Strength (RSS) measurements performed by the n nodes of a wireless sensor network (WSN). Many approaches have been considered to address this problem, see, *e.g.*, [2], but quite few consider the issue of characterizing a reliable confidence region associated to the estimated source location. In most of the cases, the Cramér-Rao lower bound (CRLB) is used to describe approximately the confidence region.

To address this problem, the *Leave-out Sign-dominant Correlated Regions* (LSCR) [1] approach is employed to define a region in the space guaranteed to contain the true source location with an arbitrary confidence level. Confidence regions as defined by LSCR are accurate even when a small set of measurements is available, but they may be non-convex or even consist of several disconnected components. Using tools from interval analysis [3], one shows that inner and outer approximations of these confidence regions may be obtained using sets consisting of non-overlapping interval vectors.

The k-th measurement obtained by the i-th node of the WSN located in $\boldsymbol{\theta}_i$ is assumed to be described by the Okumura-Hata model

$$y\left(i,k\right) = P_0 - 10\gamma_{\mathrm{P}} \log_{10} \frac{\|\boldsymbol{\theta}_0 - \boldsymbol{\theta}_i\|}{d_0} + w\left(i,k\right), \tag{6}$$

where $\boldsymbol{\theta}_0$ is the source location, P_0 is the signal power measured at some known reference distance d_0, γ_{P} is the path-loss exponent, $\|\cdot\|$ is the Euclidian norm, and $w\left(i,k\right)$ is the measurement noise. The measurement noises are assumed to be independent and symmetrically distributed. This includes the log-normal noise model usually considered.

Using the model (6), one shows that confidence regions can be obtained converging to the true source location $\boldsymbol{\theta}_0$ when the number of measurements goes to infinity provided that P_0 and γ_{P} are known. When P_0 and γ_{P} have also to be estimated, convergence is observed experimentally, even if it cannot be proved.

Comparisons of the proposed approach to maximum-likelihood and bounded-error estimation techniques are also provided.

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Non-Asymptotic Confidence Regions for Errors-In-Variables Systems

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Error-In-Variables (EIV) models in which both input and output data are contaminated by noise have applications in signal processing, image processing, and environment modeling [3]. Here, we propose a method for constructing non-asymptotic confidence region for the parameters of EIV models. The method is based on the Leave-out Sign-dominant Correlation Regions (LSCR) [1, 2].

When the input is measured without noise, LSCR constructs confidence regions by computing empirical correlation functions using different subsamples of the data set. The correlation functions are chosen such that they are equal to zero only for the true system parameters. The confidence regions are then obtained by excluding the parameter values for which the empirical correlation functions take on positive or negative values too many times since it is unlikely that any of these parameter values correspond to the true one. The constructed confidence region has the property that the true parameter belongs to it with a guaranteed user chosen probability for any finite number of data points.

An underlying assumption has been that the measured input signal is independent of the noise. This is obviously not satisfied for EIV systems, and in this talk we show how the LSCR framework can be extended to EIV models.

The data generating system we consider is

$$y(t) = \frac{B(q)}{A(q)} f(t) + e(t)$$
$$u(t) = f(t) + v(t)$$

where $A(q)$ and $B(q)$ are polynomials in the backward shift operator. $f(t)$, $v(t)$, and $e(t)$ are input, noise on input, and noise on output respectively. They are all assumed to be Gaussian. $u(t)$ and $y(t)$ are measured input and output. The models class is

$$y(t) = \phi(t)\theta + \varepsilon(t)$$

where the parameter vector θ contains the coefficients of the $A(q)$ and $B(q)$ polynomials. The regression vector $\phi(t)$ contains past output and estimated past inputs. It will be shown that, $\varepsilon(t)$ has the desired properties such that it can be used to form correlation functions from which confidence regions can be constructed.

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Regularization in Finite-Sample System Identification

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Finite-sample system identification (FSID) methods infer properties of stochastic dynamical systems under minimal distributional assumptions; typically they build confidence regions with rigorous non-asymptotic guarantees [1]. Similarly to bootstrap and Monte Carlo approaches, they generate alternative samples based on some mild regularities of the random elements of the system. An arch-typical example of such regularities is the case, when the noise sequence has a jointly symmetric distribution about zero.

Sign-Perturbed Sums [2] and, its generalizations, Data Perturbation (DP) methods [3] are recently developed FSID algorithms that can construct exact confidence regions for finite samples. They have a number of additional favorable properties, e.g., the confidence sets of SPS for linear regression problems are star convex with the least-squares estimate as a star center, as well as they are strongly consistent, meaning that the regions shrink around the true parameter, and asymptotically cannot contain false parameters (w.p.1).

Regularization is an important tool in regression which helps, for example, to handle ill-posed and ill-conditioned problems, reduce over-fitting, enforce sparsity, and in general to control the shape and smoothness of the regression function [4]. The talk will address ways to incorporate regularization techniques to FSID constructions, from standard approaches like Tikhonov regularization (ridge regression), LASSO (least absolute shrinkage and selection operator), and elastic nets to regularization with suitably chosen Hilbert space norms, which also have important applications in machine learning.

Acknowledgments This work was supported by the Nat. Research, Development and Innovation Office (NKFIH), KH_17 125698, the GINOP-2.3.2-15-2016-00002 grant, and by the János Bolyai Research Fellowship of the Hung. Academy of Sciences, BO/00217/16/6.

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Old and New Challenges in Finite-Sample Identification

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In 2005, with the publication of the LSCR algorithm (Leave-out Sign-dominant Correlation Regions, [1]), a new class of system identification algorithms for constructing confidence regions around the unknown model parameters was introduced. These algorithms had two characterising features that, together, set them apart from the previous literature in system identification: first, the constructed regions were accompanied by probabilistic inclusion results, certifying the inclusion of the true system parameters, that were rigorous for any number of data points, that is, were *non-asymptotic* in nature; second, these inclusion results were proven under very mild conditions on the noise affecting the data.

In this talk, we outline a few fundamental ideas that are at the core of LSCR and its successors, which are known under the names of SPS (Sign-Perturbed Sums, [4]), PDMs (Perturbed Dataset Methods, [5]), and, most recently, SPCR (Sign-Perturbed Correlation Regions, [3]). In the course of the presentation, the main design and application challenges in finite-sample identification will be discussed. We will also mention some recent directions of investigations in which we are directly involved; these include the relaxation of traditional assumptions such as the knowledge of the true model order, [2], and the exploitation of a-priori knowledge on the system parameters in constructing the confidence region.

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MS 30: Game Theoretic Modelling of Utility Networks

Environmentally Optimized Management of Urban Road Networks

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In this paper we address the optimal management of an urban road network by combining optimal control of partial differential equations, numerical simulation and optimization techniques [1, 2]. Specifically, we are interested in analyzing the optimal management of the intersections of an urban road network, in order to reduce both atmospheric pollution and traffic congestion.

In order to optimize the network management, we consider a multi-objective optimal control problem, balancing - within a cooperative Pareto framework - a traffic cost function involving travel times and outflows, and a pollution cost function related to contaminant concentrations.

In the second part of this work we propose a complete numerical algorithm to solve the optimal control problem, and we present several numerical tests for a real-world example of ecological interest, posed in the Guadalajara Metropolitan Area (Mexico), where the possibilities of our approach are shown.

Acknowledgments The authors thank the support from project MTM2015-65570-P of MINECO/FEDER (Spain), and from SNI-52768 and PRODEP/103.5/16/8066 (Mexico).

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Bargaining Power in the European Gas Network

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We model the European gas network as a cooperative game between countries as players over the pipeline network. We focus on the change of influence of the players in three different scenarios. We investigate how the power of the agents shift when the Nordstream pipeline is expanded, when the Ukrainian pipeline is shut down and finally when both of these happen. Although some of our findings are intuitive, there are a few slightly surprising results. One of these is that Germany is the main beneficiary of all three scenarios.

This line of research was pioneered by Hubert and Ikonnikova (2011), and Hubert and Coblani (2016). The latter analyzed the possible impact of the Nabucco and South Stream pipelines. Nothing illustrates the volatility of the gas market better than both of these projects have been abandoned since then. The latest candidate to ease Europe's dependency on Russian gas is the Southern Corridor, which aims to connect the Shah Deniz gas field of Azerbaijan to southern Europe. The success of such projects depend on many factors: how the huge costs of a new pipeline is shared, approval and legal coordination with the EU and permission of the countries whose territory is affected, to say a few. Our analysis helps to understand why the expansion of the Nordstream was pushed through by Germany and which new projects could be successful in the future.

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MS 33: Sparse and Inverse Problems in Medicine and Biology

Ultrasound Point Spread Function Estimation Using Phase Retrieval

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Blind deconvolution is a method of image resolution enhancement that seeks to estimate both the original image x and the point spread function h from the observed image y, which is modelled as $y = h * x + n$, where $*$ is the 2D convolution operator and n is additive noise. The problem needs further constraints for a unique solution. A typical approach is to define a cost function that favours sparsity of x and smoothness of h using the l_1 and l_2 norms, respectively. An alternative approach is to estimate the spectrum of h from that of y and use phase retrieval to recover h from its spectrum, using the assumptions of non-negativity and compactness [1]. Unfortunately, in the case of ultrasound imaging, h is typically highly oscillatory and non-negativity cannot therefore be assumed. However, ultrasound experiments suggest that h can be accurately reconstructed by modulating its (non-negative) envelope with a sinusoid oscillation in the depth direction, where the phase of the sinusoid modulator varies with lateral distance. Based on this observation, a so-called oscillating hybrid input-output (OHIO) algorithm was devised. OHIO is an extension of Fienup's classical hybrid input-output (HIO) algorithm [2], with the input-output step being preceded by a fixed frequency (and laterally varying phase) upmodulation; the input-output step is then followed by envelope detection. Using a set of candidate phase profiles, the OHIO estimate $\hat{h}$ is the one yielding the lowest l_1 norm $|y * \hat{h}|_1$. The approach outperforms the zero-phase estimates of h, for so long as the ultrasound images contain some locally sparse features (that is, speckle is not everywhere fully developed). This is a realistic assumption for real ultrasound images. In conclusion, the OHIO method is a promising approach to estimating oscillating point spread functions such as in the case of ultrasound imaging.

Acknowledgments M. Gyöngy was supported by the Bolyai Scholarship of the Hungarian Academy of Sciences and Grant PD 121105 of the Hungarian National Research, Development and Innovation Office (NKFIH). This work was supported by the thematic trimester on image processing of the CIMI Labex, Toulouse, France, with the Program ANR-11-IDEX-0002-02 under Grant ANR-11-LABX-0040-CIMI.

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The Influence of Source Out of Focused Grid on Image in High-energy X-ray Radiography

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Scatter radiation, which seriously decreases the precision of image reconstruction in high-energy x-ray radiography, can be largely diminished by anti-scatter grid. The anti-scatter grid model and influence under the conditions of the source out of the focused grid are studied by theoretic analysis and numerical simulation. The dependence of the direct and scatter exposures in the image plane on various grid parameters, such as aperture, distance between holes, thickness and focal length, are simulated using Monte Carlo code. Direct radiation loss fraction under the conditions such as the lateral decentering, the inclination and the source out of the focused distance are calculated by analysis. Direct radiation loss fraction under grid manufacture by the stack of foil sheets is also obtained. The theoretical results are validated using Monte Carlo code. The results are shown that the conditions of the grid out of focus toward the source and grid manufacture by the stack of foil sheets are equivalent to devalue the hole diameter, meanwhile the transmission inside the hole are held the line. The simulation results are benefited for the high-energy x-ray radiography.

Acknowledgments The authors are grateful for the support of the National Nature Science Foundation of China (Grant No. 11675021).

Pulse Diagnosis Using Arterial Blood Pressure Waveforms

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Nowadays, non-invasive diagnostic is a developing field of health care. Due to their cost effectiveness and safety, non-invasive diagnostic methods have increased importance. One emerging area in the field of cardiovascular diagnostics is pulse diagnosis. However, there is a lack of understanding about the fundamental mechanism of this method. The principle of the pulse diagnosis is that the cardiovascular system interacts with every organ in the body and therefore it delivers information about them. This information can be measured at the wrist over the radial artery based on the propagation of blood pressure (BP) wave.

Traditional pulse diagnosis relies on palpation of the pulse wave by a practitioner, hence the accuracy of diagnostic results mainly depends on the practitioner's experience. Therefore, an automatized solution is required. This pilot study introduces steps for a semi-automatized pulse diagnostic method using a novel non-invasive arterial BP measuring technique [1]. This method can record continuous BP waveform at the wrist unsupervised, and with high accuracy.

One major challenge facing automatized pulse diagnosis is filtering motion artefacts. For this purpose, a cascaded adaptive filter consisting of discrete Meyer wavelet filter and a spline estimation filter was applied, presented by [2]. For analysis the continuous BP signal has to be segmented to single-period signals. To find the segmentation points a modified version of an open source onset point detection algorithm was applied [3].

175 measurements were conducted in this study, each measurement was 3 minutes long and recorded on both hands. From the measurements waveforms for healthy, hypertensive and arteriosclerotic signals could be distinguished. Further findings could be demonstrated about how the waveform changes with age, which indicates how the arterial pressure differs due to the stiffer arterial wall.

Acknowledgments This research has been partially supported by the European Union, co-financed by the European Social Fund (EFOP-3.6.3-VEKOP- 16-2017-00002).

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Sparsity Analysis of Biochemical Reaction Networks

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Biochemical reaction networks give rise to a general class of nonlinear dynamical models (called kinetic systems) that is suitable to describe complex nonlinear phenomena not only in (bio)chemical processes but in other fields as well, where the state variables are constrained to be nonnegative [1]. We can assign a weighted directed graph to kinetic models that shows the direction and intensity of (abstract) transformations in the system. One of the main goals of Chemical Reaction Network Theory is to discover relations between the graph structure and the qualitative properties of the corresponding dynamics. The most widely known results in this context are the Deficiency Zero Theorem, the Global Attractor Conjecture [2] and the notion of absolute concentration robustness [3]. Moreover, it is a fundamental task in systems biology to reconstruct (infer) the network topology from measurement data to study possible interactions. However, it is known that the directed graph structure of kinetic models is generally not unique even if every state variable is perfectly measured. In many applications, the assumption of the sparsity of the network is meaningful and somewhat regularizes the inference problem. In [4], an algorithm was proposed to enumerate all distinct graph structures corresponding to a kinetic dynamics. In this contribution, we use and extend this approach to compute and analyze sparse structures. In our computations which are based on optimization, we allow uncertain system parameters belonging to a convex set, since these parameters are usually not precisely known in practice. We show that the sparsity assumption singificantly reduces the search space as expected, although it still does not guarantee structural uniqueness. The results are illustrated on biological examples such as metabolic networks.

Acknowledgments This research has been partially supported by the European Union, co-financed by the European Social Fund (EFOP-3.6.3-VEKOP- 16-2017-00002).

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MS 34: ECMI Special Interest Group: Big Data Models and Challenges

Statistical Analysis of the Space-Time Distribution of Cultivated Land in Lombardy Region in Italy at Parcel Level

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This work represents a preliminary attempt to evaluate ex-post impact of the common agricultural policy (CAP) *greening* payment on farmland use changes. Greening represents one of the main novelties of the current CAP programming period (entered in force in 2015), providing a horizontal payment for farmers, conditioned to the compliance with some "agricultural practices beneficial for the climate and the environment". These farm practices regard, and potentially influence, farmland allocation, particularly arable land and grassland. On this ground, we pointed our attention on analysing at a very detailed (parcel) level the temporal and spatial dynamics of farmland use transitions before and after the introduction of greening commitments. We based our analysis on a huge dataset of about 2 millions of georeferenced land parcels in Lombardy over the period 2010-2016. Crop typologies have been aggregated into 23 different categories, in order to reduce the complexity of the analysis.

The system has been modelled as a Markov chain, where each land unit evolves, from one year to the other, into one of the 23 cultivation classes. Let us denote by $p_{ij}(t)$ the probability that a land unit evolves (i.e. is cultivated) from class i to class j, from year t to year $t+1$. Our aim was to check if any statistically significant change in the transition probabilities $p_{ij}(t)$ and/or in the spatial distribution of the 23 cultivation categories, took place after the introduction of greening (that is between 2014 and 2015). Unfortunately a statistical test revealed a strong non stationarity in the $p_{ij}(t)$ for $t \leq 2014$, due to a possible correlation among data. This causes a problem in the statistical analysis, since the "physiological" variability registered before the new CAP must be filtered out for a correct comparison with the changes occurred from 2015 onwards. We solved the problem by introducing a new type of weighted χ^2 test, in which we determine the correct statistical unit that must be considered to accept the hypothesis of stationarity in a set of panel data. We applied this test to the complete set of available years (2010-2016) and we found evidence of change during 2015 in both the spatial distribution of the 23 cultivation classes and the transition probabilities of many relevant cultivations, like maize, maize for silage, wheat, soybean, etc. Furthermore we computed the Gini index to measure the heterogeneity of cultivations and the transition probabilities for the cultivation classes that resulted significant to the weighted χ^2 test. In this way we can visualise the zones of Lombardy which have mainly been affected by the greening policy.

Acknowledgments This work is supported by the project CAPTION, funded by Fondazione Cariplo, and by the Universitá degli Studi di Milano grant project 2017 "Stochastic modelling, statistics and study of the invariance properties of stochastic processes with geometrical and space-time structure in applications".

Honoring Ancestors in Matchings of Phylogenetic Trees and Ontologies

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The problem of comparing hierarchies occurs in diverse areas of biology. Phylogenetic trees or more general forms of hierarchies need to be compared to identify symbiosis between host and parasite, to evaluate tumor progression models, or to transfer knowledge from the Gene Ontology to large-scale interaction networks. In recent years, matching-based alternatives to the most popular measure of tree similarity, the Robinson-Foulds (RF) metric, have been proposed. In particular, the generalized Robinson-Foulds metric corrects some of its flaws while retaining its widely appreciated properties. Here, we build upon our previous proof-of-concept study (see [1]) and propose a method and practical software tool, Hali, that for the first time allows to efficiently compute the NP-hard generalized RF metric and variants thereof for non-trivial real-world instances. Hali combines polyhedral insights with a state-of-the-art non-linear solver to achieve an orders of magnitude speed-up and makes the generalized RF metric a "computable" distance. This allows us to systematically assess the discriminative power of our metric. In experiments on tumor progression trees we demonstrate that the tree-consistent "best corresponding node" mapping established by Hali compares favorably to traditional approaches. Finally, we extend our metric to more general hierarchies than trees (directed acyclic graphs) and compute mappings between *Saccharomyces cerevisiae* ontologies that can guide a knowledge transfer from the manually curated Gene Ontology. Our tool incorporates parallel and distributive approach in order to practically scale with real word big data instances. Hali is available at `https://bitbucket.org/mblazev/jrf`.

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Research Platform for Cyber-Situational Analysis

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Electronic information systems are used in nearly every area of life today. Besides computers smart and IoT devices turn up. However, when IT systems are used online there are cyber-threats too. The so called cyber criminals can steal unauthorised data and credentials by means of malicious codes or can have a harmful effect on IT security. If we want to observe the protection of an IT system and infrastructure against threats we must consider several relevant relating parameters. Three factors are identified in the applied model of cyber-threats – Distributed Vulnerability Assessment (DVA):

1. characteristics and prevalence of harmful cyber-threats;
2. vulnerabilities of IT infrastructure and its processes;
3. vulnerabilities deriving from users' behaviour.

There is further information of the models used for assess the risk of threats in [1] and [2].

The mentioned information are gathered using sensors from the threat landscape and using threat intelligence services these information can be extended. On the other hand IT infrastructure and users' behaviour information are collected from the IT elements in the organization. These information results a dynamic big data. In this paper the concept of a research platform is explained which can be used to perform research work on these (anonymized) data.

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Integrative Analysis of Pathway Deregulation in Obesity

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Obesity is a pandemic disease, linked to the onset of type 2 diabetes and cancer. Transcriptomic data provides a picture of the alterations in regulatory and metabolic activities associated with obesity, but its interpretation is typically blurred by noise. We solve this problem by collecting publicly available transcriptomic data from adipocytes and removing batch effects using singular value decomposition. In this way we obtain a gene expression signature of 38 genes associated to obesity and identify the main pathways involved [1]. We then show that similar deregulation patterns can be detected in peripheral markers, in type 2 diabetes and in breast cancer. Observational studies suggest that obesity might have a Mendelian origin, but it is not clear if gene expression patterns observed in obese subjects are secondary to genetic traits or not. We test our transcriptomic signature of obesity on a large cohort of twin subjects (TwinsUK). The results show that the signature correlates strongly both with the body mass index (BMI) and fat mass. Moreover in paired transcriptomes of monozygotic twins, changes in signature correlate with changes in BMI and fat mass. We also identify a set of deregulated pathways involved in obesity, from inflammation to metabolism, and show that their pathway deregulation score is strongly correlated with BMI variations in pairs of identical twins. Taken together, our results strongly indicate that alterations in gene expression observed in obese subjects are not due to their genetic background, and should therefore primarily be associated with environment and lifestyle.

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A RealForAll Project Study: Predicting Pollen Concentrations via Signal Processing and Time Series Methods

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Predicting allergenic airborne pollen concentrations is an important task for improving public health. Exposure to aeroallergens may be correlated with occurrence of allergic rhinitis and asthma, and thus it can significantly degrade quality of life and have a negative economic impact. The Interreg IPA Cross-border Cooperation project RealForAll addresses among other aspects predicting allergenic airborne pollen concentrations in the Croatia-Serbia cross-border region, where various sources of allergenic airborne pollen are present (e.g., birch trees, grass, common ragweed). In this talk, we review recent results on predicting airborne pollen concentrations based on measurements of 1) past pollen concentrations acquired through Hirst samplers and 2) a set of standard meteorological parameters. Several mathematical methods based on signal processing and time series analysis are presented and compared with conventional pollen calendar models.

Optimal Likelihood Ratio Test for Detecting Multi-State Signals

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We study detection of multi-state signals where the time that the signal spends in each of its states is of random duration. The durations are statistically described by probability mass functions assigned to each of the states. This problem finds applications in many different domains, ranging from detection of multi-state appliances (dishwasher, washing machine) from aggregate smart metering signals, and detection of pulse duration modulated signals, in engineering, to detecting marital or employment status of an individual, in econometrics. Due to the fact that the locations of state transitions are random, deriving the optimal, likelihood ratio test is in general a highly non-trivial task. By conditioning on the state transition locations, we prove that the obtained combinatorial form of the likelihood ratio test in fact admits a linear recursion representation, thus enabling computationally efficient, online testing. The matrices participating in the recursion interleave a measurement dependent diagonal matrix and a certain state-duration transition matrix of dimension linear in the maximal state duration. Finally, adopting the Neyman-Pearson criterion, we study asymptotic performance of the likelihood ratio test and derive a lower bound on the corresponding error exponent, whose tightness is then demonstrated with numerical simulations.

Massive-Scale Data Acquisition and Distributed Information Processing in Future 5g Mobile Cellular Networks

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Fifth generation (5G) mobile cellular systems are emerging as a unique platform for massive-scale data acquisition and information processing. In this work, we first review two emerging concepts critical for massive data acquisition and information processing: Machine-Type Communications (MTC) and Mobile Edge Computing (MEC). These technical concepts bring large-scale distributed information processing algorithms closer to reality and action in real-world systems [1]. Then, we demonstrate how this infrastructure can be exploited in a specific distributed information processing scenario of interest, namely, the distributed estimation problem applied to large-scale linear systems. We use the concept of factor graphs and Belief-Propagation algorithms to derive distributed algorithms that efficiently provide optimal state estimates, while being suitably matched to 5G MTC and MEC architecture [2].

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Exact Spectral Gradient Method for Distributed Optimization

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Since the seminal work by Barzilai and Borwein in 1988, and Raydan in 1990, spectral gradient methods continue to receive significant attention, especially due to their excellent numerical performance on various large scale applications. However, to date, they have not been sufficiently explored in the context of distributed optimization. In this work, we consider unconstrained distributed op- timization problems where N agents constitute an arbitrary connected network and collaboratively minimize the sum of their local convex cost functions. In this setting, we develop distributed gradient methods where agents' step-sizes are designed according to the rules akin to those in spectral gradient methods. Numerical performance of the proposed distributed methods is illustrated on several application examples.

MS 35: Reduced Order Modelling for Industrial and Scientific Applications

Prospects and Challenges of the Reduced Basis Method for Industrial Problems

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Simulation and/or optimization problems arising from industrial challenges often demand significant model reduction in particular within embedded, online or cold computing devices. We highlight some of the specific challenges within industrial projects we have been working on (e.g. from Voith Turbo (Heidenheim, Germany), Daimler (Ulm, Germany), TWT (Stuttgart, Germany)). Common issues like nonlinearities, transport dominance, lack of stability for the error/residual-relation and long-time horizons are addressed both from the practical and the mathematical point of view.

This talk is based upon joint work with S. Glas, S. Hain, M. Radic, F. Kunstmann (all Ulm), J. Brunken (Münster) and K. Smetana (Twente).

Efficient Reduced Order Simulation of Pore-Scale Lithium-Ion Battery Models

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A major cause for degradation and failure of rechargeable lithium-ion batteries is the deposition lithium (Li) as an additional metallic phase at the negative cell electrode (Li-plating). As Li-plating is influenced by the local microscale geometry of the electrode, only highly resolved models which resolve the local pore-scale geometry of the electrode will be able to faithfully capture this phenomenon. The simulation of these highly nonlinear models, however, requires significant computational resources, making model order reduction a crucial ingredient for an efficient simulation workflow.

In the interdisciplinary MULTIBAT research project we have developed such a workflow based on micrometer-scale partial differential equation models and stochastic parametrized modelling of electrode geometries, discretization using the finite volume method and, finally, reduction of the resulting discrete model using reduced basis techniques [1].

The reduced basis method (e.g. [2] and references therein) is a generic approach to parametric model order reduction based on the idea of projecting the original high-dimensional equation system onto a problem-adapted low-dimensional reduced space spanned by solution snapshots of the high-dimensional problem for certain well-chosen parameters. Unlike classical upscaling methods, this allows an efficient reduction of the computational complexity while retaining the characteristic local microscale features of the solution.

In this contribution we start with an overview of the MULTIBAT simulation workflow and give a brief introduction to the main ingredients of reduced basis methods. We then discuss the application of these methods in the context of MULTIBAT, as well as the technical realization based on our free model order reduction software library `pyMOR` [3]. Numerical examples will demonstrate the feasibility of our approach.

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ROM-Based Deflation Methods to Accelerate the Solution of Time-Varying Linear Systems

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Many applications involve the modeling of dynamical linear systems, a process that can be remarkably expensive when the simulation models are large and ill-conditioned. Therefore, several studies have been conducted to speed-up the solution of these systems.

Among others, Reduce Order Models (ROM) and deflation techniques exploit the system information to reduce the simulation computing times. Proper Orthogonal Decomposition (POD) is a ROM method where essential system information is captured on a basis, for a later reuse. Astrid et al. proposed the use of POD in an offline phase for the acceleration of problems with slightly modified parameters. Markovinovic et al. introduced the computation of a more accurate initial guess with POD methods. Making use of a POD basis, Pasetto et al. developed a preconditioner and Diaz et al. presented deflation method.

In this work, we explore the use of a ROM-based a deflation method to speed-up the simulation of flow through large-scale and highly-heterogeneous porous media with two different approaches. In the first one, we further developed the method suggested by Diaz et al., exploring the applicability of more complex systems: two-phase flow simulation including gravity and capillary pressure terms. For the second one, information is obtained in a training phase, for a later acceleration of slightly different problems.
The deflated method here presented requires from $20 - 35\%$ of the PCG iterations, i.e., an acceleration of factors up to five and it requires around $1 + \frac{p}{10}$ the number of PCG operations, for a 3D case using p deflation vectors.

We present this methodology for reservoir simulation examples, but it can be adapted to any time-varying problem, being the training phase approach particularly useful to solve problems with small variations in the parameters.

Model Reduction of Burgers Equation Using Displacement Interpolation

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We present a new numerical technique for reduction of parametrized, time-dependent nonlinear hyperbolic conservation laws in one spatial dimension. It aims to augment existing projection-based model reduction methods, by generating basis functions that are local in time and parameter. The technique builds on a simple displacement interpolation scheme based on *monotone rearrangement* [1], a scheme that arises naturally from the Monge-Kantorovich problem in optimal transport. We will demonstrate that the interpolation scheme is able to generate time-and-parameter-dependent local basis suitable for a benchmark model reduction problem involving the Burgers equation [2]. The local basis captures the behavior of the sharply localized shock-wave, as well as the globally supported source term. Mathematical justification will be given, and the extension to problems with multiple spatial dimensions will be discussed.

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Battery Modelling: Why 2D Matters

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One of the greatest challenges in developing renewable energy sources is finding an energy storage solution to smooth out the inherently fluctuating supply. Batteries provide a promising solution for this challenge, but must be managed optimally in order to maximise their lifetime. Mathematical modelling of the underlying chemical processes provides a mechanism to identify these optima. The two main modelling approaches are full physical models (such as [2]) and equivalent-circuit models. The former are computationally expensive to solve, while the latter do not provide physical insight. Our aim is to develop simplified models, based on the physical models, that provide the same insight but can be solved more efficiently and hence used for live battery management.

We use asymptotic methods, inspired by Richardson *et al.* [3], to explore a one-dimensional porous-electrode model for a constant-current discharge of a lead/acid battery and obtain a simplified model that captures all of the fundamental physical behaviour of the battery. We then investigate the more physically realistic case in which current enters the battery from the tops of the electrodes, rather than the sides, introducing a second, vertical, dimension into the model [1]. Since the aspect ratio of height to width is large, we can again use asymptotic methods to simplify the model and obtain an accurate solution much more efficiently than by solving the full two-dimensional model. By comparing the one-dimensional and two-dimensional models, we find that the impact of the vertical dimension on the voltage is significant. We compare the one- and two-dimensional models with data from lead/acid batteries provided by BBOXX, and find good agreement.

Acknowledgments VS acknowledges the support provided by the EPSRC Centre for Doctoral Training in Industrially Focused Mathematical Modelling (EP/L015803/1) in collaboration with BBOXX.

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Stability Preserving Model Order Reduction for District Heating Networks

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District heating networks are an important tool for carbon neutral urban heating due to their high flexibility towards the injection of energy. The variable energy mix combined with the dynamical thermal transport to the connected consumers makes them a challenging subject of optimization. Approaches towards finding the optimal use of the power resources such as model predictive control require simulating the network dynamics multiple times. The high number of transport pipelines and junctions in real networks of the order 10^4 makes them large scale dynamical systems, explaining the need for model order reduction. Using incompressible Euler equations, we capture the advective transport of the thermal energy within the heating network. The massflow of the transport fluid is determined by both the power requirement of the consumers and Kirchhoff's laws as nonlinear algebraic equations. Modeling the resulting massflow field as time varying parameters allows to describe the thermal dynamics as a linear parameter varying system challenging to reduce. We apply the iterative rational Krylov approximation (IRKA) to different parameter realizations and combine these to a global model of reduced order [1]. We deduce state space transformations which formulate the dynamics as a port-Hamiltonian system [2] ensuring local stability of the reduced model at every massflow parameter. The resulting low dimensional approximation adequately describes the dynamics of networks of relevant size and paves the way for optimization.

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MS 36: Mathematics in Medicine and Life Sciences

Time Reversal Methods in Acousto-Elastodynamics

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Time reversal (TR), introduced by M.Fink [1] is a subject of very active research. The principle is to take advantage of the reversibility of wave propagation phenomena, for example in acoustics, elastic or electromagnetism in an unknown medium, to back-propagate signals to the sources that emitted them.

In a previous paper [2], we introduced a time-reversed method for acoustic equation. In the present research, we solve an inverse problem in order to locate an "inclusion" (an unknown object) in an elastic medium, from partial observations of acoustic waves scattered by this inclusion. The method proposed requires developing an approach based on TR methods, to determine the elastic properties of the inclusion.

As the applications we have in mind are concerned with ultrasound-based elasticity imaging methods, we consider both elastic and acousto-elastic systems of equations. We stress that our method does not rely on any a priori knowledge of the physical properties of the inclusion.

In our talk, we will present the original method we have developed and illustrate it with some numerical results, obtained for a scatter identification problem in a layered acousto-elastic medium: this will illustrate how a scatterer can be detected and located, even in the presence of a fluid-solid interface.

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On New Proportional Controllers for Smart Bioreactors

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The new nonlocal feedback controller is used to control the production of drugs in a simple bioreactor. The mathematical model describes an enzymatic conversion of substrate into the required product. We solve a system of nonstationary nonlinear diffusion-reaction equations [1]:

$$\frac{\partial S}{\partial t} = D_S \frac{\partial^2 S}{\partial x^2} - \frac{VS}{K_M + S}, \quad (x,t) \in D = \{0 < x < X,\ 0 < t \le T\},$$

$$\frac{\partial P}{\partial t} = D_P \frac{\partial^2 P}{\partial x^2} + \frac{VS}{K_M + S},$$

where t and x are time and space variables, $S(x,t)$ and $P(x,t)$ are real valued functions. The function S defines a concentration of a pre-product (a substrate of the enzyme) and P defines the concentration of a drug (product).

We formulate two initial conditions $S(x,0) = 0$, $P(x,0) = 0$, $0 \le x \le X$ and four boundary conditions. The first three of them are classical:

$$P(0,t) = 0, \quad D_P \frac{\partial P}{\partial x}(X,t) = 0, \quad D_S \frac{\partial S}{\partial x}(0,t) = 0, \quad t > 0.$$

The last boundary condition specifies the flux of P at the boundary $x = 0$:

$$D_P \frac{\partial P}{\partial x}(0,t) = Q(t), \quad 0 < t \le T,$$

where $Q(t)$ defines the flux of the drug prescribed by a doctor in accordance with the therapeutic protocol.

The simple proportional control loop defines the changes of the substrate concentration delivered into the bioreactor at the external boundary of the bioreactor depending on the measurements of the produced drug delivered into the body and the flux of the drug prescribed by a doctor. The system of PDEs is solved by using the finite difference method. One of the most important results deals with the algorithm to select the control loop parameters. They are defined from the analysis of stationary linearized equations.

The stability of the algorithm for the inverse boundary condition is investigated. Results of computational experiments are presented and analyzed.

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A Mathematical Model for a Plant Circadian Oscilator

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Circadian rhythms are generated by intracellular transcriptional feedback loops. Recently, long non-protein coding RNAs (lncRNAs), that are natural antisense transcripts (NATs), have been emerged as novel regulators of development, disease and differentiation process in animals. In [1], a particular a circadian-regulated lncRNA, FLORE, was identified as a NAT of the CDF5 gene. In this talk we discuss a mathematical model to simulate the FLORE and CDF5 antiphasic expression in order to better understand their mutual inhibition and the relevance for the maintenance of their rhythmic expression patterns.

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Towards a Precision Ophthalmology: Targetting the Retina

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Efficacious drug delivery to the posterior chamber of the eye is a very challenging problem due to the many physiological barriers that protect the eye against the entry of exogenous substances. To avoid, or to limit, the action of these barriers several drug delivery routes are being investigated and used in clinical opthalmology. To assist medical and pharmaceutical research, mathematical modelling of the release kinetics assumes a crucial role. In this talk three dimensional computational models that simulate drug delivery from two different biodegradable polymeric platforms - intravitreal and transscleral - are presented. The models consist of coupled systems of partial differential equations linked by interface conditions, where the properties of the drug, of the implant and of the eye tissues are taken into account. Peak concentrations and residence times are compared for the two delivery routes. Particular attention is devoted to the modelling of the Blood Retinal Barrier (BRB). The influence of retinal diseases, represented by parameters that characterize the permeation through the BRB, is analyzed. Numerical simulations that illustrate the differences in the behavior of drug released from intravitreal and transscleral implants are included.

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Rational Zernike Functions Capture the Rotations of the Eye-Ball

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Zernike functions have been used with a great success in a wide range of optical, medical and engineering application areas for many decades now. The particular application area to be addressed in our proposed paper is ophthalmology. In this medical discipline, the Zernike functions are used for instance for the purpose of describing the shape – and as a consequence the optical behaviour – of the human cornea. The corneal surfaces are described in terms of the Zernike functions with the respective Zernike coefficients. The Zernike coefficients are also used for characterising and quantifying the optical aberrations of the human cornea.

Several advantageous mathematical systems – derived from the original Zernike system – were proposed in the literature. These systems have also found their way to interesting applications in the mentioned disciplines. Several discretization schemes were introduced for computing the Zernike coefficients.

The Zernike functions can be considered as representations of the Blaschke-group that describes the congruent transformations within the Bolyai-Lobachevsky geometry. Starting from the Zernike functions and making use of the Blaschke functions, a two-dimensional manifold of the rational orthogonal systems was introduced. These systems can be used to describe – or capture – the rotations of the eye-ball.

In our proposed presentation, some results concerning this representation will be shown. Application possibilities and diagnostic scenarios will be mentioned that could benefit from the aforementioned representation.

Detecting Periodicity in Digital Images by the Lll Algorithm

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Let A be a finite set of points in $\mathbb{R}^n$. A. Hajdu, L. Hajdu and R. Tijdeman [1] gave several theoretical results concerning the distance of the elements of A and shifted lattices Λ in $\mathbb{R}^n$. Furthermore, they gave an efficient method using the LLL algorithm (based upon the famous paper of A. K. Lenstra, H. W. Lenstra and L. Lovász [3]) which explicitly constructs a "well approximating" lattice for A.

A. Hajdu, B. Harangi, R. Besenczi, I. Lázár, G. Emri, L. Hajdu, R. Tijdeman [2] and A. Tiba, B. Harangi, A. Hajdu [4] gave algorithms for using this approach to detect whether some pattern components of a digital image has regular spatial distribution (i.e. they are close to some points of a certain grid). They also made computations to determine the level, where the approximation error is too large to talk about regularity, and they applied their results to the classification of typical/atypical pigment networks to recognize skin cancer.

Now we make a step further with analyzing whether a grid-like structure of points (or regions) can be considered to form a periodic pattern. For this purpose it is not sufficient that the investigated points/regions are close to the points of a regular grid; we also need to study whether the pattern contains (too many) "holes" or not. For this aim, we need some simple theoretical considerations together with the introduction of a new error measurement. We demonstrate our approach in medical image analyzes tasks, as well.

Acknowledgments Research was supported in part by the project EFOP-3.6.2-16-2017- 00015 supported by the European Union and the State of Hungary, co-financed by the European Social Fund.

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A Computational Contribution on an Ocular Iontophoretic Drug Delivery Device

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The advancement of computational technology has helped the modeling of controlled drug delivery into the biological tissues. One example is the modeling of the drug release into the human eye. Due to natural protective barriers of the eye, ocular drug delivery is considered as a major challenge in the development of treatments for diseases affecting different segments of the eye [1, 2].

In this work, the drug release from a current-mediated drug delivery device into the human eye is mathematically modeled and numerically simulated. The heat conduction, the flow of the aqueous humor in the anterior and posterior cavities are considered in the modeling. The heat distribution in different segments of the eye in the standing and supine positions is considered to study the thermal safety of the device. The effect of the voltage strength on the heat elevation of the eye segments is investigated. Numerical experiments highlight that ocular iontophoresis drug delivery system does not produce significant thermal damage and it is thermally safe for the eye.

The mechanism of the drug release from the drug reservoir into different segments of the human eye is also studied. The observations show that the drug distribution in the standing position is asymmetric while the drug distribution in the supine position is symmetric.

Acknowledgments This work is supported by Alexander von Humboldt Foundation (AvH) under the Georg Forster Research Fellowship (HERMES), hosted by Institute of Structural Mechanics (ISM), Bauhaus University of Weimar, Germany..

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Iteratively Coupled Methods for Bone Poroelasticity

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The concept of mechanically stimulated bone adaptation has been discussed extensively in the literature. In the existing models, different approaches are considered. While some authors describe this process at a cellular (microscopic) level (e.g. [3]), others investigate the bone's (macroscopic) poroelastic structure (e.g.the survey article [2]). Here we consider the application of poroelasticity theory to model of the mechanical behavior of fluid-saturated living bone tissue. We focus on the numerical solution of a coupled fluid flow and mechanics in Biot's consolidation model for poroelasticity. The method combines mixed finite elements for Darcy flow and Galerkin finite elements for elasticity. The fully coupled approach solves flow and elasticity equations simultaneously [1]. Alternatively, operator splitting techniques which decouple the pressure equation from the equation for the displacement [4], can be used for solving the discrete system. The choice of the coupling scheme affects the stability and accuracy of the numerical solutions as well as the computational efficiency. Theoretical convergence error estimates in a discrete-in- time setting will be presented for both fully coupled schemes and for iteratively coupled schemes. Numerical experiments illustrate the performance of the methods.

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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Improving Blood Flow Simulations: A Velocity Control Approach

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Vascular diseases, such as brain aneurysms and atherosclerosis, are the main cause of death in western countries. Such pathologies are not fully understood and lack precise diagnosis procedures. The mathematical modeling of blood flow in the cardiovascular system, both in normal and pathological conditions, can provide a computational tool to be used for diagnosis, prognosis or training purposes. In this sense, accurate numerical simulations must be achieved, in order to be considered reliable. However, this can be a challenge since important data, needed to close the mathematical model, are usually missing. To overcome such difficulty, optimal control techniques can be used.

In this talk, we will present possible scenarios for the application of control problems in hemodynamics, and we will discuss some mathematical and numerical aspects related to these issues.

Acknowledgments This work has been partially supported by FCT (Portugal) through the Research Project UID/Multi/04621/2013 of the CEMAT - Center for Computational and Stochastic Mathematics (at Instituto Superior Técnico, University of Lisbon), the project EXCL/MAT-NAN/0114/2012 and the grant SFRH/BPD/109574/2015.

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Effect of Aging on Transdermal Drug Delivery Enhanced by Iontophoresis: A Numerical Study

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The goal of transdermal drug delivery system is to deliver active drug molecules into the systemic circulation through the skin. The main obstacle to this approach is that the stratum corneum, the skin outermost layer, is relatively impermeable to most drugs. Several techniques have been employed to overcome this barrier. For example, one popular approach is to employ electric fields, a technique known as iontophoresis. This technique generates an electrical potential gradient that enhances drug transport across the skin [1].

The viscoelastic mechanical properties of the skin are mainly determined by collagen fibers, elastic fibers, and proteoglycans [5]. Aging has strong influence on these structures, which greatly affects the viscoelastic behavior of the skin. For instance, the elastin and collagen fibers tend to degenerate with age, which decreases the skin ability to recover from stress. Overall, these alterations induce an increase in the Young's modulus, particularly, in the stratum corneum and epidermis [3]. The aim of this study is to assess the effect of viscoelastic changes induced by aging on iontophoretic drug transport through the skin layers: stratum corneum, epidermis, and dermis. In each layer the drug transport is governed by an integro-convection-diffusion equation where the convective velocity depends on the gradient of the electric potential. The integral term accounts for the relationship between viscoelasticity and drug transport [2]. Moreover, each integro-convection-diffusion equation is coupled with an electric potential Poisson equation via Nernst-Planck relation. The numerical study is performed by means of a hybrid scheme consisting of classical finite difference and WENO finite difference schemes [4].

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Relating Barotrauma Occurrence and Hyperbaric Oxigen Terapy

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Hyperbaric oxygen therapy increases the perfusion of O_2 in tissues reducing edema and tissue hypoxia, aiding the treatment of ischemia and infection. The use of this therapy may imply some problems, being the middle ear barotraumatism the most frequent.

We intend to determine incidence and severity and to identify predictors of risk for barotraumatism of the middle ear in a large population of patients undergoing routine hyperbaric oxygen therapy.

This work studied the clinical characteristics of 1732 patients who underwent treatment at the Portuguese Navy's Center for Underwater and Hyperbaric Medicine between 2012 and 2016, in order to better characterize this issue with regard to incidence, severity and recurrence such as age, sex, clinical indication for hyperbaric oxygen therapy, personal history of allergic rhinitis and symptomatology of nasal obstruction at the time of the occurrence.

A preliminary statistical analysis was presented in [1]. In this manuscript, several statistical techniques such as analysis of variance and generalized linear models were applied. The results are interesting, but still need a more detailed 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/046 21/2013, and *Center of Naval Research* (CINAV), Naval Academy, Portuguese Navy, Portugal.

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MS 38: ECMI Special Interest Group: Material Design and Performance in Sustainable Energies

Modelling Distribution of Charge and Stress in Silicon/Graphite Anodes for Lithium-Ion Batteries

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Silicon has been found to be a very promising material for lithium-ion battery anodes due to its high capacity for lithium ions (Li^+) and is typically used in combination with other Li^+-absorbing materials such as graphite. The main problem with using silicon as an anode material is the large volume change (up to 300%) that occurs upon lithiation, causing stresses to build up in the anode, potentially leading to fracture and thus loss of capacity. In our mathematical model for this process, we consider a simple spherical particle in the anode with a silicon core and a graphite shell. We take the system to be in chemical and mechanical equilibrium to analyse both the distribution of Li^+ within the silicon and graphite, and the stresses throughout the particle. Finally, we investigate upscaling this particle model to a model of the whole anode using the method of multiple scales.

Acknowledgments This presentation is based on work supported by the EPSRC Centre for Doctoral Training in Industrially Focused Mathematical Modelling (EP/L015803/1) in collaboration with Nexeon Limited.

Mathematical Modelling for Wind Power Forecasting

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Wind power is considered among the most promising sustainable energy sources. There has been a considerable growth in the installed electricity generation capacity worldwide in the last decades. A very important issue for the successive management and exploitation of this technology, however, is the necessity of accurate forecasts for the generated power.

There exist numerous studies on methods and techniques for making forecasts on different time scales (see e.g. [1, 2] and the references therein) and the three principal approaches are the following: physically-based, statistical, and combined.

In the present work, we propose a complete procedure for predicting generated wind power, using global meteorological data, physically-based simulations of meso-scale processes, and statistically-based post-processing techniques that incorporate known local measurements.

The general methodology we use is known in the literature (see e.g. [3] and the references therein). We, however, propose some modifications of the known methods, aiming to increase the accuracy of the forecast.

Numerical experiments, based on real data, are carried to validate the applicability and accuracy of the proposed methods.

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Asymptotic Reduction of a Porous-Electrode Model for Lithium-Ion Batteries

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Lithium-ion (LI) batteries play a fundamental role in many of today's portable electronic devices and are expected to power the technologies of the future. Recent theoretical studies of LI batteries focus on using porous electrode theory to develop comprehensive models which, in principle, can guide the development of improved battery designs. However, battery optimisation is hindered by the staggering complexity of these models and the computational cost of simulating them. In this talk, we show how a systematic approach based on matched asymptotic expansions can be used to greatly simplify the governing equations. In some cases, obtain analytical solutions to the reduced model can be found. The analysis shows that the charging/discharging process can be decomposed into three main regimes and elucidates the key physical mechanisms that control battery performance. Finally, we also show that the asymptotically reduced model is able to accurately capture experimental data without the need for detailed descriptions of the physical and electrochemical parameters.

Acknowledgments This work was funded by an Irish Research Council New Foundations Grant.

Modeling Microstructures for Light Harvesting Surfaces

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In this talk the topography of nanostructures consisting of arrays of crystalline Si (c-Si) nanodots is discussed. We present formulations for interfacial energy settings that support partial wetting and grain boundaries to predict the equilibrium morphologies of silicon nanodots and compare them to experimental results. We then present an anisotropic phase-field model and corresponding sharp-interface model that describe the dynamics of the dewetting process towards the nanodots.

Steering pattern formation during dewetting with interface and contact lines properties

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Self-assembly using dynamic pattern formation processes provides an important toolbox that enables cost-efficient large-scale industrial manufacturing of microstructures. In order to be able to tune the pattern formation process in a desired direction, it is important to understand how to influence occurring patterns using physical parameters of the dynamic process. Dewetting of thin liquid layers is a process, capable of creating droplet patterns on microscopic and mesoscopic length scales with different underlying physics, *e.g.* see [1, 2]. The underlying mathematical model for the conserved quantity $h(t,\cdot):\Omega\to\mathbb{R}$ is

$$\partial_t h - \operatorname{div}\left(m(h)\nabla\tfrac{\delta E}{\delta h}\right)=0, \qquad E(h)=\int_\Omega \tfrac{1}{2}|\nabla h|^2 + W(h)\,\mathrm{d}x,$$

where the process can be tuned with the non-negative mobility $m(h)$ or with the driving (free) energy functional $E(h)$. We show how dewetting from a solid surface can be influenced by modifying the properties of the nanometric surface layer by tuning the magnitude of friction at the liquid-solid interface [3, 4]. We discuss the physical significance of tuning interfacial properties, highlight the underlying modeling philosophy, and show its practical impact using numerical simulations.

Acknowledgments This research of DP is carried out in the framework of MATHEON supported by the Einstein Foundation Berlin.

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On Accurate Optical Simulations for Solar Cells

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Photovoltaics is the fastest growing technology for sustainable electricity generation. To facilitate further growth of the technology, high power conversion efficiencies are required. Hence, it is critical to maximize the fraction of the incident sunlight, which can be harvested.

Optical simulations are pivotal to increasing the understanding of the interaction between sunlight and solar devices. The specific demands of the complex optical systems under investigation combined with the stochastical properties of sunlight pose challenges for a simulation method.

We show how the finite element method (FEM) can be employed in an application example to simulate nanostructured solar cells. With FEM periodically nanotextured devices can be simulated rigorously [1, 2]. We also how a thick glass superstrate on top of the device can be properly taken into account [3]. Further, we will discuss how advanced optimization algorithms can be deployed in a meaningful way. As an example, we discuss results of a recent optimization study for perovskite-silicon tandem solar cells [4].

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MS 39: Towards the Next Generation of Digital Human Modelling

Fiber-Based Modeling of Muscles in the Musculoskeletal System

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The aim of this contribution is to present a fiber-based modeling approach for the dynamic behavior of muscles within the musculoskeletal system. We represent the skeletal system as a rigid multi-body system which is actuated by muscles. Various models for the muscular force generation with different levels of details can be found in literature. Many models relay on Hill-type force elements incorporating passive and active muscle activities [1]. Such models are computational effective but do not represent the real situation accurately. In contrast to Hill-type models, 3D representations of muscles allow for the inclusion of mass, large deformations, incompressible material behavior, complex geometries, fiber orientations, local activation principles and chemo-electrophysiological aspects [2, 3]. However, such models come along with an increased computational cost and increased modeling complexity.

In the present approach, we model each muscle fiber bundle as a 1D cable with variable cross section undergoing large deformation and strains. We employ an incompressible Neo-Hookean material for the passive behavior and a active stress law found in the literature [2]. We incorporate contact between the fiber bundles with a finite element framework by a penalty method. We apply our framework to conduct a forward simulation of a upper limb model.

Acknowledgments The authors are grateful for the support of the Federal Ministry of Education and Research (grant W123456).

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Reinforcement Learning in Order to Control Biomechanical Applications

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In order to solve an optimal control problem a bunch of techniques are well studied and understood. In the last years techniques belonging to the research field Artificial Intelligence (AI) gain in importance in the optimal control field. One of the most famous techniques in this field is Reinforcement Learning (RL) [1]. It is shown, that RL can be used to learn how to play Atari games [2], to beat professional players on the game Go (summarized in [1]) and many more examples for successful applications of RL are available.

In this talk, we introduce the RL as a technique in order to control biomechanical systems. The functioning is demonstrated by applying RL to a simple model of a human arm. This biomechanical system consists of three rigid bodies (upper arm, lower arm and hand). The bodies are connected by three joints, which are represented by black dots in Figure **??**. Furthermore, the system is equipped with Hill's muscles [3] in order to control the system. Hill's muscle is a simple model of a muscle and its structure is sketched in Figure **??**. In our biomechanical example (Figure **??**) it is represented by a red line.

We define a suitable goal for the human arm (i.e. move the hand to a requested position) and afterwards we show how the result computed by RL looks like. The results and the advantages of RL may motivate to apply this technique to more complicated biomechanical system in the future.

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Multi-Obstacle Muscle Wrapping Based on a Discrete Variational Principle

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Simulations of biomechanical multibody systems actuated by Hill-type muscles are established as a major tool for investigating human motion. In addition to the activation level, typically, muscle actuated systems require to compute muscle paths, their length and their rates of length change to determine the muscle force. In particular, the muscle force direction is influenced by the muscle path. Assuming that the muscles are always under tension, their path is often modelled as a locally length minimizing curve that wraps over moving obstacles representing anatomical structure of the human body [1].

This work is based on a mechanical analogue to find the shortest path on general smooth surfaces, using a discrete variational principle [2]. In this context, the geodesic path is reinterpreted as the force-free motion of a particle in n dimensions under holonomic constraints. The muscle path is then a G1-continuous combination of geodesics on adjacent obstacle surfaces. It can be described as a shortest path boundary value problem with G1-continuous transitions across a certain number of obstacles [1, 3, 4].

This contribution focuses on the technical details of the proposed method for multiple obstacles, while specific biomechanical applications will be presented in the future. In the given form, the formulation avoids nested loops and is well suitable to be used in an optimal control framework based on the direct transcription method DMOCC (Discrete mechanics and optimal control for constrained systems [5]). Examples show the application of the given wrapping method to a certain number of general smooth surfaces.

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Optimal Control Simulations of Lateral and Tip Pinch Grasps

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Grasping is a basic, though complex human movement performed with the hand through its many degrees of freedom. During grasping, when the hand closes around the object, the multibody system changes from a kinematic tree structure to a closed loop contact problem. To better understand work-related disorders or optimize execution of activities of daily living, an optimal control simulation to perform grasping is useful.

We simulate the grasping action with a three-dimensional rigid multibody model composed of two fingers (the thumb, described in [1], and the index finger) along with the wrist and the forearm, modelled with the discrete null-space method, see [2]. The model is actuated using joint torques. The grasping movement is composed of a reaching phase (no contact) and a grasping phase (closed contacts). The contact constraints are imposed first using functions to calculate the distance between the finger tips and the object surfaces and then through spherical joints. The durations of each phase is determined by the solution of an optimal control problem. Thus, the dynamics is described by a hybrid dynamical system with a given switching sequence and unknown switching times. The closed-loop dynamics are adopted from [3]. The optimal control problem is solved using the direct transcription method DMOCC (discrete mechanics and optimal control with constraints), see [4], leading to a structure preserving approximation. An objective function involving either the contact polygon centroid, the grasp matrix or the contact force is minimized subject to the discrete Euler-Lagrange equations, boundary conditions and path constraints. The dynamics of the object to grasp along with Coulomb friction is also taken into account. Investigations are done for two examples, namely lateral pinch and tip pinch grasps.

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MS 40: HU-MATHS-IN: Applications in the Life Sciences

The Impact of Vaccination on the Spread of Varicella in Hungary

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Varicella is one of the most common infectious diseases of children, which can be prevented by vaccine. Varicella causes not only the chickenpox of children, but also the herpes zoster at an older age. In Hungary, the vaccine is marketed for more than 15 years, but it has been obligatory only from this year. Unfortunately, there has been hardly any study neither on its impact nor the effectiveness of different vaccination strategies.

In our talk, we consider age-structured models of varicella infections including vaccination strategies taking into account the Hungarian specialties. We perform parameter estimations and verifications for the different models, do predictions and investigate the cost-effectiveness of of the models.

Acknowledgments This research is supported by the EU-funded Hungarian grant EFOP-3.6.2-16-2017-00015.

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Combining Convolutional Neural Networks and Hand-Crafted Features in Medical Image Classification Tasks

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In the recent years, convolutional neural network (CNN) based deep learning approaches have been demonstrated an amazing performance in several digital image processing prob- lems compared with traditional ones [1, 2]. An essential factor in the dominance of CNNs is that these methods extract the features involved in the solution of the task through a learning process opposite to traditional approaches, where the features are usually pre- defined by human experts – the latter type of features are also called hand-crafted ones. However, in this work we present that a suitable arrange of traditional and CNN features into an ensemble framework may still lead to further improvement, since they can have diverse behavior. As a general approach, we describe how the features of more CNNs and traditional extractors can be combined in such an architecture that can be optimized by theoretical tools of machine learning. A basic principle of ensemble learning is that the inclusion of more diverse members can be expected to better performance. To implement this idea, we also suggest a complementary technique to make the feature extractor mem- bers of such architectures more diverse by including a penalty term [3] in the loss function to suppress correlation in the optimization process.

The efficiency of our approach is demonstrated in several medical image analysis tasks. Namely, experimental results for the classification of dermoscopy and retinal images and the localization of corresponding lesions are presented proving that the mixture of tra- ditional [4] and CNN features in machine learning scenarios is currently a competitive approach.

Acknowledgments Research was supported in part by the projects GINOP-2.1.7-15- 2016-01641 and EFOP-3.6.2-16-2017-00015 supported by the European Union and the State of Hungary, co-financed by the European Social Fund.

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Dynamics of Novel Delay Logistic Equations from Cell Biology

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The delay logistic equation, originating from Hutchinson, has played a crucial role in the theory of nonlinear delay differential equations, inspiring the development of a variety of methods. However, the equation has received criticisms from biological modellers due to the lack of a mechanistic derivation. In this talk we present a new delay logistic equation with clear biological underpinning from cell population dynamics, motivated by the go or grow type behaviour of glioma cells. First we construct some individual based stochastic models under different biological assumptions, where the cell cycle length is explicitly incorporated, and investigate their behaviours.

Then the mean field equations are derived, and they turn out to be logistic type delay differential equations with discrete and distributed delays. For the most challenging case, we provide a complete global analysis of the equation showing global asymptotic stability of the positive equilibrium, based on persistence argument, comparison principle and an L2-perturbation technique. Yet, the dynamics is not trivial, as there exist very long transients with oscillatory patterns of various shapes, for which we offer some explanations.

We also show that if we add an instantaneous positive feedback term to the classical delay logistic equation, then local stability does not imply global stability so a Wright-type conjecture is not valid any more (this last part is from a joint work with István Győri, Veszprém and Yukihiko Nakata, Shimane).

Model Diagnostics and -Specification for Epidemiologic Models

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The residual diagnostics [1] of the statistical models often used in epidemiology (e.g. Poisson or negative binomial regression [2] with longitudinal dimension) is often convoluted. Complicating factors include nonlinearities [3], testing of residual autocorrelation – due to the longitudinal dimension –, possible interactions between different levels of time (such as different long-term trend in different days of week) and stratification according the important factors, such as sex and age. The present paper overviews these challenges, and illustrates the possible ways to solve them on a real-world dataset consisting of more than 10 years of follow-up data on several interventions – lower limb amputation [4], myocardial infarction, cataract surgery etc. – from a nationwide administrative database in Hungary.

Acknowledgments The authors are grateful for the support of the HU-MATHS-IN project, number: EFOP 3.6.2-16. Tamás Ferenci is supported by the ÚNKP-17-4-I-OE-779/71 New National Excellence Program of the Ministry of Human Capacities.

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MS 41: ECMI Special Interest Group: Computational Methods for Finance and Energy Markets

Implementation of Agglomerative Clustering and Genetic Algorithm in Portfolio Optimization

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Creating and managing a successful stock portfolio is a difficult and challenging practice caused by the uncertainty created by the fluctuation of the stocks and the randomness in the market itself. Portfolio diversification, as stated in modern portfolio theory, is the go-to solution for managing risks. The purpose of portfolio diversification is to reduce the return's variance compared with a single stock investment or undiversified portfolio. The primary motivation of this research is to investigate the portfolio selection strategies through clustering and application of genetic algorithm. Clustering serves as a method to cluster assets with similar financial ratio scores (the scores of EPS, PER, PEG, ROE, DER, Current Ratio and Profit Margin). Through use of the clustering method, homogeneous clusters are produced and can be used in diversifying portfolio. In this research, Agglomerative Clustering is used as the clustering method. Genetic Algorithm will then be applied to each resulting cluster to obtain the optimal proportion of each stock in the portfolio. The Genetic Algorithm is built based on the Mean-Variance Cardinality Constrained Portfolio Optimization model, hence making it a Constrained Genetic Algorithm. The performance of Constrained Genetic Algorithm refined with Agglomerative Clustering in portfolio optimization, which is evaluated based on some actual datasets, gives a portfolio that beats the market and has bigger expected return than a portfolio constructed with only Genetic Algorithm or a portfolio constructed by uniformly weighted stock.

Acknowledgments The authors are grateful for the support of the PITTA UI 2018 Grant.

A Simple Market Coupling Model with Reserve Allocation and Minimum Income Condition Bids

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As the proportion of renewable sources is increased in the power mix, the uncertainties related to generation also do increase. System operators use reserves allocated on ancillary service markets to ensure the safe operation of power systems under such uncertainties, and uncertainties originating from demand. Joint energy and reserve markets [2] allow the simultaneous allocation of power and reserve production. These markets support those power plants who are able to produce reserves in the vindication of their market power. On the other hand, the recently introduced concept of minimal income orders [1] provides a possibility for plants to submit their bids taking into account their technological constraints and costs more explicitly. If such markets are connected, the clearing algorithm has to consider transmission bottlenecks regarding power and reserves as well [3].

In this paper we analyze a simple example where joint energy and reserve markets allowing minimum income condition bids are coupled, and propose a possible approach for the clearing of such markets.

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A Stochastic Price Model for the German Secondary Balancing Power Market

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A modeling approach for the German secondary balancing power market is proposed. Individual bids in the pay-as-bid auction are modeled separately. The offered capacity and energy price are modeled by their empirical distributions. Due to the complex structure and incomplete information from market data, the capacity price is assumed to follow a Gaussian mixture model, which has to be estimated on truncated data [1]. A calibration algorithm is proposed, which is applied to publicly available data from the German market. The calibrated model is used in a simulation study for a cost analysis of the whole market. Moreover, bidding strategies of an individual market participant are evaluated with respect to the distribution of her potential returns. The results can contribute to the ongoing debate on changes of the German market design [2].

Acknowledgments P. Oktoviany is grateful for the financial support from the Fraunhofer Society for the Advancement of Applied Research.

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Multilevel Price Estimation of Jump-Diffusion Driven Assets

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In this talk, we introduce a jump-split scheme for which the time-stepping can be chosen independently of the jump times, implying that the computational complexity of the method is independent of the jump intensity for Merton type jumps. We combine this method with the Multilevel Monte-Carlo (MLMC) method introduced by Giles [2] and show that using the Milstein scheme and the antithetic approach suggested by Giles and Szpruch [3] combined with the *weak* MLMC introduced by Belomestny and Nagapetyan [1] results in second order variance reduction and thus also quadratic computational complexity in the mean square error (MSE). These theoretical results are confirmed by numerical experiments applied to jump-diffusive assets.

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High-Order Methods for Parabolic Equations in Multiple Space Dimensions for Option Pricing Problems

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In this talk we discuss higher-order spatial discretization methods using finite differences and pseudo-spectral methods and demonstrate how to use it in a sparse grid combination technique. Next, for the time discretization we propose alternating direction implicit (ADI) schemes and analyse its stability.

We conclude with two applications to financial engineering partial differential equations: Basket-Options in the Black-Scholes model and European Plain-Vanilla options under Stochastic Volatility.

For related work we refer the interested reader to [1, 2, 3, 4, 5].

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Hysteresis Due to Irreversible Exit: Addressing the Option to Mothball

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This paper analyses the following hitherto understudied feature in real switching options: a firm has a mothballing option and an option to permanently abandon. If the firm finds itself in an operating mode with a price just above the abandonment threshold, it is unclear whether to exercise the abandonment option or to exercise the mothballing option. If the price goes down, the firm may exit, but, surprisingly, if it goes up, it may mothball. In that case, we prove the existence of an hysteresis region, where the firm stays in production, with negative prices.The paper discusses in which cases, depending on relations between the involved costs and the diffusion parameters, the firm decides to exit or to mothball. There needs to be jumps in the stochastic profitability driver in order to ever ending up in the hysteresis/waiting region while in a producing mode.

A Multi-Step Spline Scheme for Solving Backward Stochastic Differential Equations

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In this work we study a multi-step scheme on time-space grids for solving backward stochastic differential equations. We use spline interpolating polynomials to approximate the time-integrands, which are conditional expectations, with values of the time-integrands at chosen multiple time levels. The resulting scheme is a semi-discretization scheme in the time direction involving conditional expectations, which can be then numerically solved using the Gaussian quadrature rules and polynomial interpolations on the spatial grids. Several numerical examples including applications in finance are presented to demonstrate high accuracy of the multi-step scheme.

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Weak Approximation of Index-Linked Catastrophe Bond Prices

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We consider the subject of approximating tail probabilities in the general compound renewal process framework, where severity data are assumed to follow a heavy-tailed law (in that only the first moment is assumed to exist). By using the weak convergence of compound renewal processes to the α-stable Lévy motion [1], we derive such weak approximations. Their applicability is then highlighted in the context of an existing, classical, index-linked catastrophe bond pricing model [2], and in doing so, we specialize these approximations to the case of a compound time-inhomogeneous Poisson process. We emphasize a unique feature of our approximation, in that it only demands finiteness of the first moment of the aggregate loss processes. Finally, a numerical illustration is presented. The behavior of our approximations is compared to both Monte Carlo simulations and first-order single risk loss process approximations and compares favorably [3].

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High-Order Scheme for Option Pricing with Stochastic Volatility and Jumps in Returns

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Option pricing remains an interesting area of study for mathematicians driven by the demand for financial derivatives among traders and investors alike. We introduce a IMEX high-order compact finite difference scheme to compute options priced under the Bates Model, [1]. The Bates model is a stochastic volatility model which allows for jumps in returns, posed by coupled stochastic differential equations we are able to apply standard derivative pricing arguments to obtain the PIDE

$$\frac{\partial V}{\partial t} + \frac{1}{2}S^2\sigma\frac{\partial^2 V}{\partial S^2} + \rho v\sigma S\frac{\partial^2 V}{\partial S\partial\sigma} + \frac{1}{2}v^2\sigma\frac{\partial^2 V}{\partial\sigma^2} + (r-\lambda\xi_B)S\frac{\partial V}{\partial S} + \kappa(\theta-\sigma)\frac{\partial V}{\partial\sigma} - (r+\lambda)V + \lambda\int_0^{+\infty} V(S\tilde{y},v,t)p(\tilde{y})\,\mathrm{d}\tilde{y}.$$

Following the method employed by Salmi and Toivanen, [4], we accomplish the implicit-explicit discretisation in time by means of the IMEX-CNAB method, defined as

$$(L_D)\,u^{n+1} = \left(L_D + \frac{3}{2}L_I\right)u^n - \left(\frac{1}{2}L_I\right)u^{n-1}.$$

To achieve high-order convergence we utilise the finite difference scheme used by Düring, Fournié, [2], to implicitly compute the differential operator, L_D, while we evaluate the integral operator L_I explicitly using Simpson's rule. The scheme is coded in C++ with use of the GSL libraries.

In addition to a discussion of the methodology, we will present the results of numerical experiments, which examine the convergence and stability of the scheme. We will also discuss how this new high-order scheme can be beneficial to financial practioners interested in hedging options using the Greeks, as discussed in [3].

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Applications of the Heston Stochastic Local Volatility Model in Commodity Markets

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Stochastic Local Volatility (SLV) models have become the industry standard for FX and equity markets. The local volatility extension of the popular Heston stochastic volatility model is a promising candidate within the zoo of SLV models. The Local Volatility component of the Heston SLV model allows for a natural modelling approach of the Samuelson effect, which is prevailing in commodity markets. In addition, the stochastic component assures consistent pricing over the entire volatility skew. The presentation introduces a multi-factor Heston SLV model for the forward curve dynamics in conjunction with a day-ahead process including potential spikes. An efficient calibration algorithm together with a fast and accurate simulation scheme allows for fast pricing of Asian averaging, multi-callable/Bermudan-style options, which are common in gas markets.

European Gas Prices Dynamics: EEX, Ad-Hoc Study

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This paper regards the dynamics of gas spot prices on one of european energy exchanges - EEX. A detailed description of the price dynamics is provided alongside with several multi-factor models allowing to forecast daily gas prices. An original approach to the development of such multi- factor daily price models is proposed. Specifically, daily price models taking into account non-integer power of time variable tend to perform better on the horizon of several weeks. A descriptive analysis of the data also gives new qualitative insights into european gas prices dynamics.

The Trade-Off Between Liquidity and Correlation: Proxy Hedging of Bunker Fuel

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Fuel costs are a substantial component of the shipping industry, making bunker fuel price risk a major consideration for shipping firms. We analyse the hedging effectiveness of different proxy hedges with oil futures as well as OTC forwards for the bunker fuel market. Using different hedge ratios and a VECM-GARCH modeling approch it is found that oil futures' hedging effectiveness has significantly improved over the past 20 years. Despite this improvement, in the minimum-variance framework, the forward contracts' higher correlation still yields better hedging results. However, given the high amount of transaction costs for OTC products, the exchange-traded oil futures contracts can deliver higher mean-variance utilities and can thus be considered a viable candidate when hedging fuel for ships. We explore the tradeoff between liquidity and correlation that dominates this important energy market challenge.

MS 42: Evolutionary Game Theory with Time Constraints (in Biology and Medicine)

The Replicator Equation in Matrix Games Under Time Constraints

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We are now interested in how the monomorphic ESS is related to the existence and stability of equilibria for polymorphic populations. We point out that, although the ESS may no longer be a polymorphic equilibrium, there is a connection between them. Specifically, the polymorphic state at which the average strategy of the active individuals in the population is equal to the ESS is an equilibrium of the polymorphic model.

In the casewhen there are only two pure strategies, a polymorphic equilibrium is locally asymptotically stable under the replicator equation for the pure-strategy polymorphicmodel if and only if it corresponds to an ESS. Finally, we prove that a strict Nash equilibrium is a pure-strategy ESS that is a locally asymptotically stable equilibrium of the replicator equation in n-strategy time-constrained matrix games.

Evolutionary Stable Strategies in Matrix Games with Time Durations

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Game theory focuses on payoffs and typically ignores time constraints that play an important role in evolutionary processes. For instance, Holling-type functional response takes into account that the number of active predators is less than their total number, since after a successful attack predators have to handle and digest their prey before they continue hunting. Moreover, in optimal foraging theory, in ecological games on kleptoparasitism, and in the dispersal-foraging game, time constraints have an essential effect on optimal behavior.

Following our paper [1], we introduce matrix games with time durations, where each pairwise interaction has two consequences: both players receive a payoff and they cannot play the next game for a specified time duration. Thus our model is defined by two matrices: a payoff matrix and an average time duration matrix. Maynard Smith's concept of evolutionary stability is extended to this class of games. First, we derive formulas for the players' average payoff via heuristic calculation under two assumptions, then we introduce an exact mathematical model, where those requirements are met and the heuristic calculations get justified with rigorous proofs. For that we assume that the waiting times are exponentially distributed, thus we can use the standard method of continuous time Markov processes to describe the stationary state of the population. Finally, we illustrate the effect of time constraints by the well-known prisoner's dilemma game, where additional time constraints can ensure the existence of unique evolutionary stable strategies (ESS), both pure and mixed, or the coexistence of two pure ESS.

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Several Characterizations of ESS of the Matrix Game Under Time Constraints

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Evolutionary stable strategy (ESS) is a central notion of evolutionary game theory introduced by Maynard-Smith and Price for classical matrix games [3]. This is an uninvadable strategy in the sense that a population of individuals of this strategy resists mutants appearing in a small enough amount. Recently, Garay et al. introduced a game theoretic model with time constraints [2] and analyzed its relationship with the equilibrium points of the replicator dynamics [1]. We give some static and dynamic characterizations of ESS under time constraints which are analogous to those for classical matrix games.

Acknowledgments The first author's research was supported by the EU-funded Hungarian grant EFOP-3.6.1-16-2016-00008. This project has received funding from the European Union Horizon 2020: The EU Framework Programme for Research and Innovation under the Marie Sklodowska-Curie grant agreement No 690817 (to J.G. and T.V.).

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MS 44: Recent Mathematical and Statistical Approaches in Earth and Environmental Sciences

Simulating the Air Temperature of the City of Novi Sad, Serbia

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The simulation of air temperature is of concern in agriculture, in the energy sector, for water management, in the environmental business, and in many other industries. Thereby, it is essential to correctly model the variation of daily air temperature and especially the differences between individual measuring stations, i.e., locations. This knowledge helps e.g. farmers to calculate the risk of frost in April or an energy company to estimate the photovoltaic production, which – among other things – depends on the temperature.

Besides setting up an adequate temperature model one also needs to tackle the problem of data quality, i.e., missing data and measurement errors. The aim of this research is to analyze preprocessing methods and modeling concepts for high-dimensional multivariate temperature data using the city of Novi Sad, Serbia, as an example. Here we have a number of stations measuring temperature in ten different zones distinguished only on the basis of their physical properties. First, in order to improve data quality, a new dynamic preprocessing algorithm for anomaly detecting is developed. In the next step, we propose a new clustering scheme based on temperature data which divides the city into seven clusters. The measured data of each cluster's temperature stations are averaged and aggregated to the daily level. Different time series models like the sparse vector Markov switching autoregressive models and the seasonal vector autoregressive model are tested to find a proper model for simulating daily temperature. In the second step, granularity is increased and the simulation is done on an hourly level.

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Stochastic Order Relations in Various Environments

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First we will introduce a multivariate joint lifetime model, where the whole dependence structure is based on modifications of univariate exponential distributions. Namely, we assume that the original lifetime parameters $\lambda_1, \lambda_2, \ldots, \lambda_n$ of the institutions will be modified as $\lambda_i + a_{ji}$ $(i = 1, \ldots, n, i \neq j)$, when the default of institution j occurs. This model enables a very flexible dependence modelling due to the fact, that for each pair (i, j) there is a parameter a_{ij} defined. Our work is partly motivated by the well-known Marshall-Olkin model, which is also established on modifications of exponential distributions. However, while the Marshall-Olkin distribution allows common shocks for subsets of entities (which is not typical in banking systems), in our suggested model we deal with cascading effects, where the default of a particular institution affects the remaining lifetime of (some) other institutions. Our model also includes the Marshall-Olkin type models as a special case.

We present the fundamentals of our lifetime model as well as some interesting properties of the multivariate copula which stems from the model. We investigate – under a symmetric parameter setting – the monotonicity of our copula in certain copula orderings, especially in the convex order and increasing convex order, as the parameter of the copula varies. Then we relate our copula model to the quantification of systemic risk in financial systems.

As a further example, we will show another, quite different environment, where stochastic order relations can be proved between some naturally arising random variables. Namely, we are interested in exploring the structure of lottery type gamblings by finding advanced indicators that stem from the distribution of random variables which are associated with the corresponding game. Our work is motivated by a standard 90/5 type lottery setting. The outcomes in this particular game are described by five-tuples, and we consider the ordered sample of these outcomes, and investigate (among others) the ordered differences between the neighbouring elements of the ordered sample with respect to the increasing convex order (Lorenz order). We illustrate our results by a data set obtained from Hungarian lottery history from 1957 to 2018. In addition we will examine a natural continuization of the above setting, which possesses nicer mathematical properties than the original discrete one. We will prove Lorenz order relations between some appearing quantities. Finally we present some ideas for possible extensions.

Damage Margin Calculation for Extreme Natural Disasters

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Many environmental processes may lead to extreme risks or critical damage (e.g. heat waves, storms), resulting in huge financial losses. One can model such data using extreme value theory. The related statistical methods aim to estimate the parameters of interest, most importantly the tail of a distribution, which is determined by the so-called tail index parameter. The tail of of a regularly varying distribution function F can be written as $1 - F(x) = x^{-1/\xi}\ell(x)$, where $\ell()$ is a slowly varying function and ξ is the tail index parameter. One of the widely used estimators for the tail index is the Hill estimator, which is based on the k upper order statistic. Finding the optimal k is an important research question, which was investigated by recent works [1], [2].

We realised (see [2]) that the proposed method results in biased estimators when the tail index $\xi > 0.5$ and the sample size is less than 10 000. Here we proposed a consistent method which reduced the bias. It turned out that our approach is suitable for estimating the tail index for all realistic cases. The bootstrap plays an important role in the procedure.

We investigated two main types of natural disasters in Europe: extreme temperatures and storms, based on the data EM-DAT [3], which consist of losses from the last 100 years. After the analysis by the proposed method, we can say that both the damage of temperature and storm has high (> 0.5) tail index parameter. In the talk we shall compare our method with more classical approaches like the maximum likelihood and present estimates for the return values (high values) of the environmental catastrophes in Europe.

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Optimal Groupings and Inhomogeneity Detection in Environmental Sciences and Beyond: Examples of the Combined Cluster and Discriminant Analysis (CCDA) Method

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Some research questions in environmental sciences sparked the development of new statistical methods of general applicability. An example is the combined cluster and discriminant analysis (CCDA) method [1]. CCDA can be used for finding the optimal grouping of sampling sites in a monitoring network [2], as well as for detecting very small differences between sub-groups of sampling sites [1, 3, 4]. Obtaining such information about the system can be particularly useful for the optimization and planning of current monitoring networks. While in environmental sciences sampling sites (or even periods of time) are the sources of data, CCDA could be used far beyond, in any setup, where multiple multivariate samples are available from different sources and the goal is to group these sources optimally or to detect inhomogeneities. The corresponding software is available in R [5].

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Interpolation Using Different Combinations of Environmental Observations

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The state of our environment is monitored in order to enable a quantitative description of its state and in order to reduce the potential risk of adverse events. In most cases measurements are taken at different times and locations. Traditionally these measurements were taken at selected point locations and interpolation/regression methods were used for interpolation. The development of new sensors and the availability of other related information makes the revision of these techniques necessary. Categorical data and interval type measurements (detection limit problem) are among others important challenges. In this contribution possibilities to combine different types of data is discussed. Methods based on rank statistics and copulas are presented. Examples from hydrometeorology and regional groundwater quality mapping illustrate the methodology.

Utilizing the Periodic Behavior of Water Quality Parameters in Estimating Primary Production in a River

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The development of models to estimate environmental variables is especially important in aquatic systems, e.g. where measurements of primary production are lacking. Morlet wavelet spectrum- and multiple linear regression analyses were conducted on 15 water quality variables sampled at 14 monitoring sites along the Hungarian section of the River Tisza and 4 sites from artificial tributary channels for 1993-2005. Interestingly, the presence of annual periodicity was found to vary over space and time. In general, an increase was observed in the company of higher trophic states of the river heading downstream. Water quality variables were combined into 7 different groups (nutrients, ions, etc.) and their periodicity indices were computed. By exploiting their spatial distribution along the studied river section, multiple regression models were derived. In the models the periodicity indices of the groups of water quality variables served as independent-, and the proxy of primary production (chlorophyll-a) served as the dependent variable. In fine, an improved model was constructed which was capable of explaining about half (adjusted $R^2 = 0.5$) of the variance of primary production in the study area.

Acknowledgments The authors are grateful for the support of the Bolyai János Scholarship.

MS 45: Optimization

Pickup and Delivery with Time Window Uncertainty

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We consider dynamic pickup and delivery problems with time window uncertainties as defined recently by [1]. In that model there is a transportation service provider that gets calls from customers with exact pickup and drop-off locations, but with inaccurate estimations of the time windows for the transportations. The time windows of the service requests become known with certainty only after a second call from the customers, shortly before the service may start. There are several real-world scenarios where the above uncertainty is predominant.

We present a new algorithm that may help transportation service providers that operate in the above context to find better vehicle tours. Our method is based on estimating the expected operational costs, where missing a customer request is heavily penalized, and the other cost component is the total deadhead cost (operating empty while going to the next pickup location or to the depot). The novelty of our approach is that unlike [1], we do not generate scenarios, and we solve only a single minimum cost flow problem at each decision point, while [1] solves several MIPs at each decision point (one for each scenario).

Yet, our method outperforms their method in terms of average total cost on several classes of instances with various characteristics, while it is inferior only in a well-characterized setting. Another advantage of our method is its low running time, the entire simulation run with 100 customers and 40 vehicles was less than a second. The exact solution of the same instance with perfect information and large desired time windows was frequently more than 20 minutes on a modern notebook. This would prohibit the application of scenario based approaches which would repeatedly solve MIPs, as the solution time of a single MIP would be too large, not mentioning that for a large number of customers, one may have to consider much more scenarios than [1] did on their 20-customer instances.

Acknowledgments This work has been supported by the National Research, Development and Innovation Office (NKFIH), grant no. K112881, and by the GINOP-2.3.2-15-2016-00002 grant of the Ministry of National Economy of Hungary.

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Optimizing Majority Voting Based Systems Under a Resurce Constraint for Multiclass Problems

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Generating ensembles from multiple individual classifiers is a popular approach to raise the accuracy of the decision. As a rule for decision making, majority voting is a usually applied model. In this paper, we consider a variant [1] of classic majority voting, which incorporates probability terms $p_{n,k}$ to constrain the basic framework. These terms control whether a correct or false decision is made if k correct votes are present among the total number of n. In this work, we extend this model with adding a natural resource constraint in terms of a time limit within which the ensemble should make the decision. For this aim, we consider both the execution time t_i and accuracy p_i of each member, where the value of p_i is considered as independent and identically distributed random variables. Then, we solve the problem on how to find the most accurate ensemble, where the sum of the execution times of its members remains below the limit. More specifically, the aim is to compose an ensemble, which maximizes the constrained ensemble accuracy

$$q_T = \max \left\{ \sum_{k=0}^{s} p_{s,k} \left(\sum_{I \subseteq K, |I|=k} \prod_{i \in I} p_i \prod_{j \in K \setminus I} (1-p_j) \right) \middle| K \subseteq M, s = |K|, \sum_{j \in K} t_j \leq T \right\},$$

where the time T is given, and $M = \{1, 2, \ldots, n\}$.

The above optimization task leads to a non-separable Knapsack problem, which is addressed by a novel stochastic approach based on the estimation of the joint behavior of the members. Our methodology can be applied to various tasks, like for the localization of the optic disc in retinal images [1], pattern recognition [2], neural network ensembles [3]. As a practical demonstration for the efficiency of our approach, we present empirical results for medical image analysis and human resource management tasks.

Acknowledgments Research was supported in part by the project EFOP-3.6.2-16-2017- 00015 supported by the European Union and the State of Hungary, co-financed by the European Social Fund.

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B&C for Scheduling with Raw Material Constraints

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Machine scheduling with raw material constraints has a great practical potential, as it is solved by ad-hoc methods in practice in several manufacturing and logistic environments. In the talk we present an exact method for solving this problem with the maximum lateness objective based on mathematical programming, our main contribution being a set of new cutting planes that can be used to accelerate a branch-and-cut (B&C) based mathematical programming solver.

More formally, we focus on scheduling a single machine subject to raw material constraints. That is, in addition to the machine, there are some raw materials with an initial stock and some additional replenishments over time with a-priori known dates and quantities. Jobs may require various quantities from these resources, and a job can be started only if the required amount is on stock. Upon starting a job, the stock level of all the resources are decreased by the quantities needed by the job. Each job has a due-date and the objective is to minimize the maximum lateness. As an illustration, consider the figure below depicting a schedule of two jobs on a single machine, and notice that job J_2 must wait until the replenishment of the raw-material at date u_2 occurs, because the first scheduled job decreases the stock level below its requirement.
We will discuss modelling issues, and then after fixing a particular MIP formulation, we will present inequalities valid for the set of feasible solutions, and also some that may cut off feasible, but not optimal solutions.

We will also summarize computational results on a wide variety of instances.

Acknowledgments This work has been supported by the National Research, Development and Innovation Office (NKFIH), grant no. K112881, and by the GINOP-2.3.2-15-2016-00002 grant of the Ministry of National Economy of Hungary.

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Pairwise Comparisons in Multi-Criteria Decision Making

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Multi-attribute decisions form an important class of decision problems, since the selection of the best action(s) is based on multiple and often conflicting criteria. The decision maker's preferences can be modelled and quantified by the method of pairwise comparisons. Missing comparisons occur in a natural way in real decision situations, especially if the number of items to compare is large. The incomplete version of two well known methods, namely the eigenvector method [4] and the logarithmic least squares is uniquely solvable if and only if the graph of comparisons is connected [2]. Pareto optimality (efficiency), the key concept of multiple objective optimization, plays an important role in weighting. A weight vector is called Pareto optimal if its pairwise ratios approximate the matrix elements, filled in by the decision maker, such that the approximations cannot be improved without making it worse in at least one position. Recent algorithms detect inefficiency and find a dominating Pareto optimal weight vector [1].

Pairwise Comparison Matrix Calculator [3], developed by the Research Group of Operations Research and Decision Systems, Laboratory on Engineering and Management Intelligence, Institute for Computer Science and Control, Hungarian Academy of Sciences (MTA SZTAKI), is a free online tool for calculating weights from incomplete pairwise comparison matrices as well as for efficiency analysis.

Acknowledgments The author is grateful for the support of the Hungarian Scientific Research Fund (OTKA, grant no. K111797), and the János Bolyai Research Fellowship of the Hungarian Academy of Sciences (grant no. BO/00154/16).

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MS 46: Environment Modelling and Remote Sensing by Computational Imaging

Segmentation and Change-Detection of Remote Sensing Images Using Fusion-MRF Model

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Classifying segments and detecting changes in terrestrial areas are important and time-consuming efforts for remote sensing image analysis tasks, including comparison and retrieval in repositories containing multitemporal remote image samples for the same area in very different quality and details. We propose a multilayer fusion model for adaptive segmentation and change detection of optical remote sensing image series, where trajectory analysis or direct comparison is not applicable. Our method applies unsupervised or partly supervised clustering on a fused-image series, followed by multilayer Markov random field (MRF)segmentation. The resulted label map is applied for the automatic training of single layers. After the segmentation of each single layer separately, changes are detected between single label maps [1]. The proposed method has been numerically validated on remotely sensed image series with ground-truth data, including Wetland mapping in multi-temporal multispectral satellite imagery [2]. The workflow of the proposed ML-FMRF model with the short description of its main processing steps are illustrated in Fig. 4.

Acknowledgments This work was supported by OTKA/NKFIH No. 120499.

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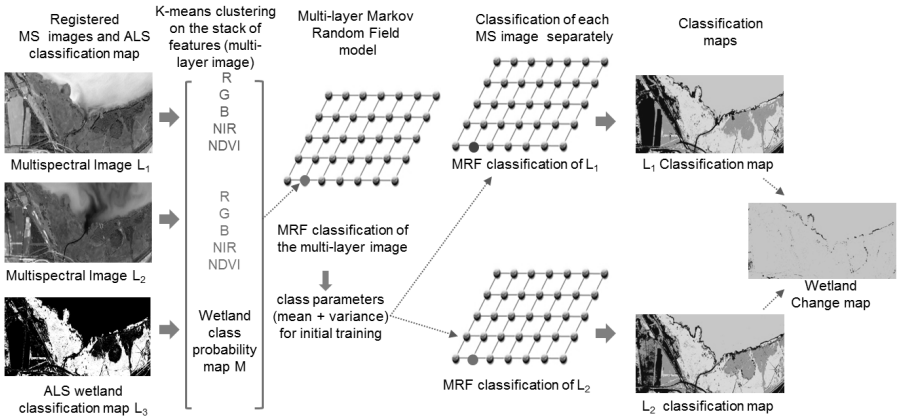

Figure 4: Workflow of Multi-Layer Fusion MRF classification and change detection [2]

Point Cloud Based Vegetation Habitat Quality Assessment Using Fuzzy Classification

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Sustaining the Natura 2000 protected habitat network in the EU costs approximately 5.8 billion EUR per year, with inadequate management estimated to cause 450 billion EUR of loss in opportunity costs[1, 2]. Assessing habitat status and quality is a complicated process that requires quantification and evaluation of multiple variables such as vegetation structure, patchiness, the presence of characteristic species, soil and water conditions and human management. Remote Sensing is expected to play an important role in streamlining and upscaling the monitoring process, but so far it has not been possible to observe such complexity in sufficient detail [3]. Meanwhile, Airborne Laser Scanning (ALS) coverage of European countries is rapidly increasing, with 17 EU member states now having full datasets of their area and many regions have already been scanned in several consecutive years. Airborne Laser Scanning is a three-dimensional surveying method that measures position and radiometric properties of target objects with centimeter accuracy in decimeter-sized footprints. Typically up to 100000 measurements are made each second in a near-equidistant scan pattern, resulting in a set of points with densities ranging from 1-50 points every square meter. We aimed to develop a method for quantifying habitat conservation status according to Natura 2000 monitoring guidelines in high resolution based on ALS. Our study area was an alkali grassland vegetation mosaic in the Hortobágy National Park. In order to represent the smooth transitions and continuously varying vegetation composition in this grassland, we had to use fuzzy classification and develop our own remote sensing data analysis software based on random forest machine learning [4, 5]. The advantage of this approach was that spatially explicit accuracy analysis was possible and the setup of categories and training and evaluation datasets could be optimized. We also developed a novel indicator for fuzzy class accuracy and proved the connection to the widely used confusion matrix indices. The class probabilities obtained from fuzzy classification proved to be especially useful since they were found to be related to species composition and the intensity of local damage to the habitat. ALS-based proxies were successfully defined for each of the variables required by the official mapping scheme, and each proxy was calibrated based on ground truth samples. Finally, a GIS scheme was designed that calculated a weighted sum of these variables based on the scoring system laid out by the field guidelines. The final output was a map of 8000 000 pixels with 0.5 m resolution and a complete Natura 2000 conservation status assessment for each unit. Based on independent evaluation data, it was found that the final score is correct in 80 % of the cases. This methodology produces habitat status maps with substantial added value compared to only field-based mapping, and allows rigorous evaluation of accuracy and representativity.

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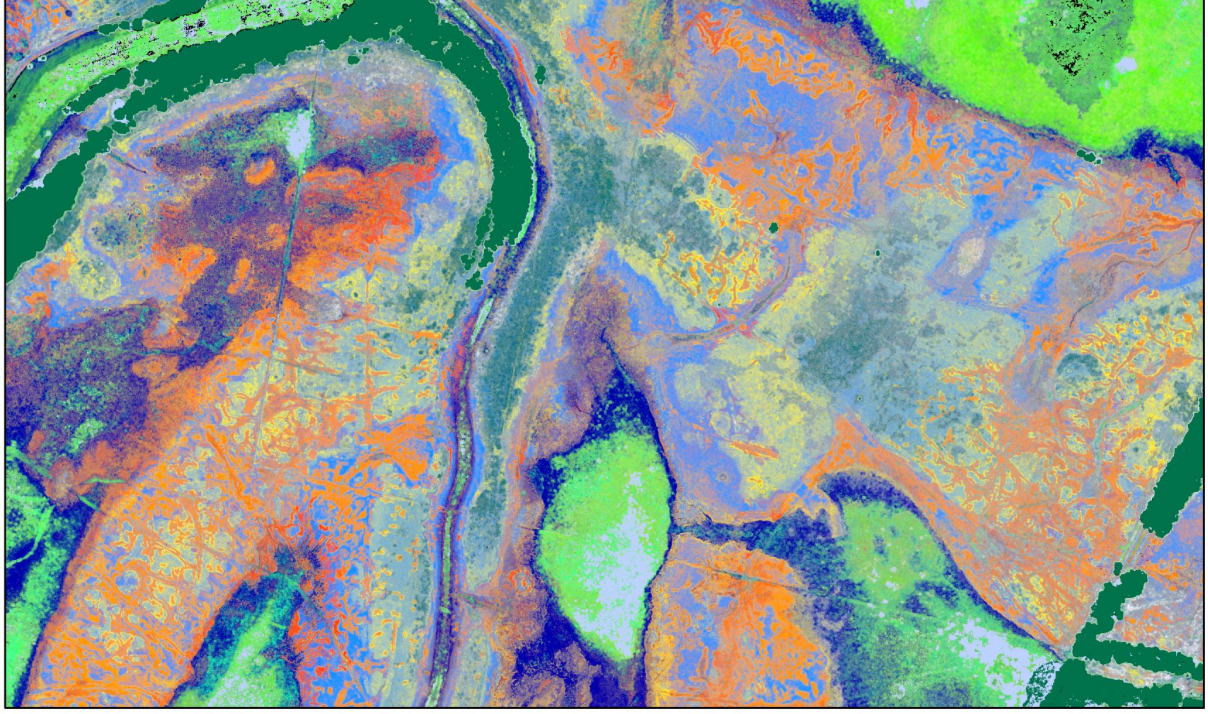

Figure 5: Cutout of the fuzzy habitat map of the study area, where the individual colours represent different grassland vegetation classes. Note smooth transitions and detailed patterns corresponding to micro-topography features.

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Relative Pose Estimation of Omnidirectional, Perspective and Lidar Camera Systems

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A methodology is presented for the relative pose estimation of a camera - 3D lidar pair without the use of any special calibration pattern or point correspondences. The method has no specific assumption about the data source: plain depth information is expected from the lidar scan and a central projection camera (both traditional perspective or omnidirectional) is used for the 2D images. The calibration is solved as a 2D-3D registration problem using a minimum of one (for extrinsic) or two (for intrinsic-extrinsic) planar regions visible in both cameras. The registration is then traced back to the solution of a non-linear system of equations which directly provides the calibration parameters between the bases of the two sensors. The method has been tested on a large set of synthetic lidar - camera image pairs as well as on real data acquired in outdoor environment. The method has been succesfully applied for 3D modeling in Cultural Heritage.

Acknowledgments This work was partially supported by the NKFI-6 fund through project K120366; "Integrated program for training new generation of scientists in the fields of computer science", EFOP-3.6.3-VEKOP-16-2017- 0002; the Research & Development Operational Programme for the project "Modernization and Improvement of Technical Infrastructure for Research and Development of J. Selye University in the Fields of Nanotechnology and Intelligent Space", ITMS 26210120042, co-funded by the European Regional Development Fund.

MS 47: Mathematical Modeling of Charge Transport in Graphene and Low Dimensional Structures

Chaotic Behavior and Coherence Resonance in Semiconductor Superlattices at Room Temperature

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Random number generators (RNG) are key in many areas: data security, numerical simulations, online games of chance, etc. Classical generators can be either insecure or slow. Recent solutions that avoid both problems include doped weakly coupled semiconductor superlattices which, operated at room temperature [1] can produce spontaneous chaotic oscillations. This can be exploited to generate true random numbers fast enough and with little post-processing.

Under DC voltage bias, idealized superlattices [2] show self-sustained chaotic behavior for certain voltage intervals. If external and internal noise is taken into account, these voltage intervals can be made broader and the chaotic response enhanced. Thus, establishing superlattices as a robust physical entropy source.

Another feature seen both in experiments [3] and numerical simulations [4] is coherence resonance: external band limited voltage noise of sufficient amplitude induces regular current self-oscillations in states that are stationary in the absence of noise. Furthermore, when a weak AC voltage signal is applied, coherence resonance triggers a stochastic resonance. That is, the current response is both phase locked to the AC signal and amplified, in the sense of a higher signal to noise ratio.

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Hybrid Parallel Deterministic Solver for DG-MOSFETs

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The simulation of Double Gate MOSFETs is of interest from the point of view of techno- logical development, because transistors are the building block of any electronic device. From the practical point of view, simulations spare trial-and-error lab experiments. Deterministic solvers have the advantage over Monte-Carlo solvers, much used by the com- munity of engineers, of properly describing almost-empty zones of the device and of being noise-free. Among the deterministic solvers, we have chosen to make simulations using a very accurate but in exchange very time-consuming Boltzmann–Schrödinger–Poisson solver, as introduced in [1]. Then, in order to improve the performances, the code has been parallelized on the CPU using MPI [2]. Here, we present our prelimirary results on a hybrid CUDA-OpenMP parallel implementation of the solver on GPU-CPU.

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Charge and Phonon Transport in Graphene

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Both kinetic and macroscopic mathematical models for charge and phonon transport in graphene are presented. The first ones are represented by semiclassical Boltzmann equations which are solved with a Direct Simulation Monte Carlo approach or with a discontinuous Galerkin scheme. The macroscopic models are obtained by the moment method with closure relations de- duced by the application of the maximum entropy principle. Quantum correction are also included with the aid of the Wigner formalism. Simulations for suspended graphene and for graphene on a substrate are shown. In view of possible applications of graphene on electron devices, several issues are addressed, in particular the importance of the interband scattering and the crystal heating due to the charge flow.

Asymptotic Study of Quantum Transport in Low Dimensional Nanomaterials

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Recent years have witnessed a surge of interest for the electronic properties of low dimensional nanomaterials. Such nanomaterials show remarkable transport properties due to the peculiar structure of the energy band spectrum. The confinement of the electrons in thin sheets induces relevant quantum effects that modify the usual transport mechanisms.

It is generally challenging to develop a framework capable of reproducing two important aspects of the nanomaterial physics: the coherent quantum mechanical evolution of the system and the loss of quantum coherence due to collisions. The coherent quantum evolution of atom and electrons is described by reversible Hamiltonian dynamics. Collisions are a complex many particle effect and are usually treated at the level of classical mechanics. The development of new methods for the simulation of complex systems, has a wide array of potential applications.

In this talk I will present some recent results that concern the application of multiscale models to the electron transport in nanomaterials. The model that I will discuss includes some important aspects of the quantum dynamics and is capable describe relaxation effects. In particular, I will focus on the so called interband tunneling transition process. Such a phenomenon describes the quantum tunneling of a particle (electron or hole) induced by an external field which is supposed to be strong. The relevant quantum tunneling concerns the transfer of charge between regions of the energy spectrum which are completely separate in the usual adiabatic limit.

Charge and Energy Transport in Graphene

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A hydrodynamical model for the description of the charge and the energy transport in graphene is presented. The state variables used for the physical system are moments of the electron and phonon occupation numbers, and their evolution equations are derived by integration from the respective Boltzmann equations. The closure of the system is obtained by means of the maximum entropy principle (MEP) and all the main scattering mechanisms between electrons and phonons and among phonons themselves are taken into account. Numerical simulations are presented in the case of a suspended graphene monolayer.

Multiscale Modelling for Materials Science Applications

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Multiscale modelling is nowadays a general trend in computational physics and industrial mathematics, as it allows the numerical simulation of complex processes and phenomena that would be otherwise impossible to study solely by means of first principles approaches. Within this framework, a simplified problem is initially investigated through accurate calculations and appropriate parameters are extracted. Thereon, these parameters are used to calibrate theoretical models that are computationally less demanding whilst able to span in space- and time-scales that are comparable to those of real processes and experiments. A particular case regards the simulation of mass and electron transport. In this case, the atomistic mechanisms and related parameters can be investigated and calculated accurately in the quantum framework of the Density Functional Theory (DFT) and DFT-based Molecular Dynamics (MD). Indeed, *ab initio* approaches guarantee the theoretical evaluation of the atomic properties of materials specifying their constituents (atoms and electrons), without any relevant approximations. The integrated development of simulation codes supported by *ab initio* quantum calculations can significantly improve the quality of the transport models and the portability of their parameter calibration. The basis of the predictability potential for the mathematical model derives from the proper matching of the DFT/MD calculated "information" (e.g. material parameters, atomic configuration, migration/diffusion paths, energetics, electronic structure, etc.) in the simulation schemes. The calibrated simplified approaches can then efficiently simulate large systems for long times, i.e. at the scale of interest for the experimental studies. In this presentation we will discuss examples from our studies for such coupled numerical techniques, considering the cases of graphene [1, 2] and hybrid perovskites [3].

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On a Thermodynamically Consistent Coupling of Quantum System and Device Equations

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In this talk we discuss a hybrid modeling approach for the coupling of the classical energy-drift-diffusion models for carrier transport in optoelectronic devices to quantum mechanical based microscopic models.

These hybrid models are thermodynamically consistent: the conservation of the energy and positive entropy production are preserved. The physical structure of the problem is well separated into reversible effects, driven by the free energy, and dissipative effects, driven by an entropic gradient system.

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About Concept of the Finite Element Package ACELAN-COMPOS for Active Composite Materials Simulation

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The ACELAN-COMPOS package is intended for computer design of two-phase active composite materials with the coupling of mechanical and electromagnetic fields. The most common class of such materials is the class of magnetoelectric composites. In these composites, one phase is a piezoelectric with the coupling of mechanical and electric fields, and the other phase is a piezomagnetic with the coupling of mechanical and magnetic fields. Thus, due to the general coupling through the mechanical fields, the composite acquires an additional magnetoelectric connectivity. Other widely used examples of active composites are the piezoelectric composites consisting of a piezoelectric phase of one basic material and a piezoelectric or elastic phase of another material (possibly pores).

In order to determine the effective moduli of such composites, a comprehensive approach is used, which includes the effective moduli method, the modeling of various structures of representative volumes, and the finite element method. This technology is implemented in the currently developed package ACELAN-COMPOS. The ACELAN-COMPOS package is developed by a large number of researchers, some of whom are listed as authors of publications on ACELAN-COMPOS in recent years [1, 2].

This work describes the models of magnetoelectric composites, which take into account the size effects; the methods for creating representative volumes, based on the types of connectivity of the composite and the peculiar properties of its internal structure; and the homogenization methods and the basic units of ACELAN-COMPOS. We provide the examples of the representative volumes simulation for the granular composites, for the composites with the coupling of both phases and some other types of two-phase composite structures. The results of solving the homogenization problems for porous piezoelectric composites and for piezoelectric composites with elastic inclusions are also presented. In these calculations, the representative volume models generated in ACELAN-COMPOS were then transferred to the ANSYS finite element package, where the effective moduli of the composite were calculated. In future, the full cycle of calculations is expected to be carried out in ACELAN-COMPOS package. Future prospects for the development of the ACELAN-COMPOS package are discussed in conclusion.

Acknowledgments The author is grateful for the support of the Ministry of Education and Science of the Russian Federation, project No. 9.1001.2017/4.6.

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A Monte Carlo Algorithm Without Time Discretization Error for the Wigner Equation

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The Wigner transport equation represents a promising model for the simulation of electronic nanodevices, which allows the comprehension and prediction of quantum mechanical phenomena in terms of quasi distribution functions. The development of Monte-Carlo algorithms for this quantum kinetic equation have been tackled, using a a probabilistic model based on a particle system with the time evolution of a piecewise deterministic Markov process [1, 2]. Each particle is characterized by a real-valued weight, a position, and a wave-vector. The particle position changes continuously, according to the velocity determined by the wave-vector. New particles are created randomly and added to the system. The main result is that appropriate functionals of the process satisfy a weak form of the Wigner equation. Moreover, a stochastic algorithm without time discretization error can be introduced. The approximation error and the efficiency of this algorithm are discussed in benchmark test cases [3].

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Charge Transport in the Three-Dimensional Topological Semimetal Cd3As4

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The three-dimensional topological semimetals, like Cd_3As_4, are characterized by the presence of a 3D Dirac-like node, which can be approximated by a cone with vertex in $(k_x, k_y, k_z) = (0, 0, k_0)$. Thus, only at $k_z = k_0$ the in-plane dispersion is a gapless Dirac cone, while for other parallel planes the nonzero term $k_z - k_0$ plays the role of an effective mass term, producing a gap in the in-plane dispersion relation. We present a macroscopic model for charge transport in Cd_3As_4 based on the Maximum Entropy Principle.

MS 48: ECMI Special Interest Group: Towards a Virtual Campus in Industrial Mathematics

European Net Portal for Industrial Mathematics

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Online environments are a viable media to access dispersed knowledge and support innovative processes, training and educational needs, consultation, etc. We envisage a possibility to build a European digital environment and web-portal for applied and industrial mathematics. An ECMI Special Interest Group was formed to work towards e-courses and in longer perspective an IM learning portal.

Such environment would be suitable for students in applied mathematics and engineering programs and also for persons already in working life who are looking for continuing education and professional development. ECMI has almost 30 year history of collaboration in sharing experience and building an educational programme in industrial mathematics. The pooled expertise provides a foundation for a versatile, high quality and up-to-date content production representing forefront-knowledge.

If at first 4-6 active ECMI nodes joins the group, and each will design and brings to the portal 1-2 special courses or course modules (3-10 ects) emerging form their local strengths and specializations, we would already have a significant educational resource.

The course topics would reflect current research and forefront knowledge having relevance and demand in the industrial R-D and in educating industrial mathematicians or research scientists. The value for the R-D community is up-to-date material, which is not yet available in abundance in commercial media. The merit of the courses might be on a customised content for a special applications area. The asset feature being the design and the usability for a certain target group of users.

One potential use for such learning resource would be international exchange, double degree cooperation and educational knowledge alliances. An example could be collaboration with the developing countries, where the availability of up-to-date special courses in applied mathematics is poor and the shortage of academic staff is a severe obstacle for developing an applied math programme with relevance to real world applications. A web portal of good courses with fresh and up-to-date content would be a big asset for them. So-called virtual mobility can be integrated as a component of an exchange programme and real mobility. The department offering the courses for remote users should be able to provide local tutoring in order to exploit the web-course portal in an efficient way.

ECMI Modeling Course: Blended Learning in Applied Mathematics

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"Virtual education" is one of the main keywords when it comes to 21st century teaching. However, the definition of this term ranges from providing lecture slides online to mobile phone app development. Education in mathematics, in particular, still has a high affinity to chalk-and-blackboard lectures as well as closed solutions (proofs) of problems. Albeit in their later career outside the university environment, many students have to deal with imperfect data sets from real-world problems. To prepare future industrial mathematicians for this challenge, we designed the "ECMI Modeling Course" on applied mathematics.

Blended Learning in Applied Mathematics: Within a special interest group (SIG) on virtual education, we built up a Moodle-based online platform to bring the knowledge and methodology of all participating partners together. In detail, the members of the SIG were the University of Koblenz, Lappeenranta University of Technology, Tampere University of Technology, University of Verona, St. Petersburg Polytechnic University, University of Coimbra and University of Lisbon. Each partner processed and provided one real-world problem on late Bachelor's or early Master's level. Data and MatLab codes as well as video lectures could be accessed by students from all participating institutions. A local supervisor served as functional contact and communicator in case of occurring problems.

Blended Learning in Applied Mathematics: Some of the advantages of our online course compared to classical lectures are

1. the applicability of mathematical methods to real-world data,
2. the increased motivation of students for finding solutions,
3. the variety of methodology used by each partner, and
4. the experience of the often misused term "mathematical modeling".

Our talk gives an overview over the course, presents the problems addressed, assesses selected student solutions and discusses possible continuations and enhancements for future releases.

Beanstalk: Russian Contribution to ECMI Virtual Education Program

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The educational program in Applied Mathematics at Institute of Applied Mathematics and Mechanics (IAMM) of St. Petersburg Polytechnic University is emphasized at various aspects of computational mechanics. By joining ECMI virtual education program IAMM intended to examine and to adopt the methods of virtual and remote training used by ECMI colleagues and also to present the educational approaches used in IAMM.

The most challenging part of the project was choosing and adaptation of short modelling course that is meant to fit our area of scientific interests and also has some national specifics. The idea was suggested by short Science Fiction novel Jak and the Beanstalk by Richard A. Lovett [Analog Science Fiction and Fact, v131 # 7 & 8, July/August 2011]. The story is about a guy who climbs the tower (Beanstalk) that is 65000 kilometers high. The novel mentions that such tower makes it possible to launch shuttles to Mars using just centrifugal force with minimal additional energy.

The students were proposed to conduct a technical audit of Beanstalk project as it was described in the novel. It turns out that the task can be considered from different points of view and various modeling approaches can be used on different levels: from analytical solutions of ordinary differential equations to advanced finite element analysis.

The whole task generally exceeds two weeks of work scheduled in the ECMI modeling course. However it demonstrates basic principles of work with industrial projects. The task was divided into several problems with increasing complication. Some basic problems were recommended as obligatory part, while the rest of the problems were posed as optional ones.

The presentation is to be devoted to illustration of educational program in Applied Mathematics at IAMM by example of Beanstalk course and summation of our participation in ECMI virtual education test program.

Experiences and Modernization on Online Courses in the Finnish National Network on Mathematical Modelling

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The Finnish National Network on Mathematical Modelling was founded by the following Finnish universities and their departments: Lappeenranta University of Technology, School of Engineering Science; Tampere University of Technology, Department of Mathematics; University of Eastern Finland, Department of Applied Physics and Department of Physics and Mathematics; University of Jyväskylä, Department of Mathematical Information Technology and the University of Oulu, Department of Mathematical Sciences. The departments share their interest and experience in mathematical modelling in order to develop and use mathematical methodology to solve important problems in science, economics and industry. The main activities of the network consist of modelling, simulation, collaboration with industry and society, in terms of projects, modelling weeks and study groups.

The departments spread across Finland have joined their forces to teach mathematical modelling. The purpose has been to offer students a chance to study mathematical modelling and to utilize what has been taught earlier on various mathematics courses, but what has frequently not been sufficiently integrated, to direct students' thoughts to real world problems and to teach them how to use simulation software to solve small scale problems. As joint teaching would be impossible in a classic lecture room setup due to long distances between universities, the departments took their teaching to the Internet. This was pioneer level work done before the times of Youtube, social media or other tools that are commonplace today. As an outcome, web-based learning and teaching methods as well as content production methods for mathematical modelling have been developed.

The courses offered include the Basic Course in Mathematical Modelling (5 ECTS) and multiple advanced courses from different topics, each worth 4 ECTS. The basic course is intended for second and third year students who already have experience in the basics of matrix algebra, ordinary differential equations, numerical analysis, probability theory and statistics. The advanced courses include Continuum Models, Soft Computing Methods of Mathematical Modelling, Modelling and Optimization and Modelling with Partial Differential Equations. Two advanced courses are offered annually. Over a thousand students have completed these courses as a part of their studies in engineering and mathematics.

With the rise of MOOCs and online multimedia and with the experience of many years of online teaching, the FNNMM has decided to review the best practices and teaching methods to be used on the courses. Also, a revised version of the course is being designed in English. This presentation aims to (1) qualitatively present the course walkthrough and the workload of the teachers and students, (2) describe and share the best practices found when designing a national level, multi-institutional course in mathematics, and to (3) describe the plans and methods for modernization of the course to make better use of the tools and skills available today, compared to the late 90s.

MS 49: Knowledge Discovery and Graph Data Science

On Branching Strategies for Exact Maximum Clique Search

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The Maximum Clique Problem is a fundamental NP-hard problem in graph theory which finds numerous real-life applications spanning a variety of disciplines, such as computer vision, planning, robotics, coding theory, network analysis or bioinformatics. In the last decade an important number of algorithmic improvements concerning its exact solution under the branch-and-bound paradigm have been proposed. The relevance of these improvements is shifting the attention of researchers to solve other fundamental combinatorial problems and applications by reducing them to a maximum clique problem. In this talk, some of the cutting edge improvements concerning exact maximum clique search will be discussed [1, 2, 3, 4], including iterative Russian Doll enumeration and infra-chromatic bounds. Also subject of this talk will be specific tailoring techniques for massive real-world graphs [5].

Acknowledgments The author is grateful for the support from the Spanish Ministry of Ecnonomy and Competitiveness (grant DPI2017-86915-C3-3-R).

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Network Analysis with NetworKit - Interactive and Fast

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Network analysis is increasingly applied to study various real-world phenomena, where dealing with large graph data sets comprising millions or billions of edges has become mandatory. In order to analyze such massive data, we need algorithms whose running time is nearly linear in the number of edges. However, many methods that are deemed successful on small networks, are quickly limited when the network size increases significantly. Therefore, developing a scalable analysis tool suite that includes fast variants of such methods is crucial. Here we present NetworKit [4], an open-source software suite for processing and analyzing large networks. We describe our methodology to develop scalable solutions to network analysis problems, including parallelization, fast heuristics for computationally expensive problems, efficient data structures, and modular software architecture. NetworKit is implemented as a hybrid, combining performance-critical parts in C++ (using OpenMP for parallelism) with an interactive Python user interface.

The package provides a wide and growing range of functionality, including common and novel analysis algorithms and graph generators. Focus areas include community detection [1], structure-preserving sparsification, and the centrality measurements [2]. Our fast generators create graphs that exhibit typical complex network structure (e. g. random hyperbolic graphs [3]), meant for scaling studies and benchmarking purposes. Also, NetworKit exploits the correspondence between graphs and matrices (GraphBLAS, `http://graphblas.org`) and has been used for supporting probabilistic range queries in large spatial data sets. In experiments on networks with millions or billions of edges, the ratio of graph size and running time is usually between 10^6 and 10^8 for NetworKit's nearly-linear time algorithms. Compared to the closely related software packages graph-tool and igraph, NetworKit shows consistently highest performance.

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Job Sequencing and Clique Search

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The job sequencing problem is an optimization problem. Certain products are to be produced on given machines satisfying predetermined technological order. The objective is to determine the sequence of jobs in which the various products are processed on the machines in the least possible time. The well-known standard approach recasts the problem by means of mixed integer linear program. Here we experiment with a more combinatorial idea.

Given a positive number T we construct an integer k and an auxiliary graph G. The graph G encodes the constraints of the job sequencing problem. If the graph G contains a k-clique (a clique with k vertices), then there is a feasible job sequencing whose completion time is at most T. So, instead of an optimization problem we are dealing with a decision problem.

The practical utility of the clique search framework is three fold. A greedy sequencing procedure can be used to locate a feasible but typically far from optimal job sequencing. The difficulty of the clique search problem depends on the parameter T. If T is near to completion time of the greedy schedule, then the k-clique problem is relatively easy. As T gets closer and closer to the completion time of the optimal schedule the clique search problem gets computationally harder and harder. The k-clique search version of the job sequencing problem can be used to locate a not optimal but feasible solution that out performs the simply greedy sequencing. The k-clique search can be carried out in a parallel fashion in a relatively straight-forward manner. Finally, there is technique due D. Knuth which allow to estimate the the size of the search tree of a k-clique locating algorithm. So we have an indication if the clique search we are attempting is cost effective or not.

It must be clear that the k-clique search version of the job sequencing problem will not always be a competitor of the standard mixed integer programming reformulation. Rather it is a complementary technique which maybe useful when one needs a not necessarily optimal feasible solution.

An Improved Maximum Common Subgraph Solver

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Maximum common subgraph problem is used in chemistry as a means of comparing shapes of molecules, either as 3D scans or molecular graphs, which represent the structural formula directly. An example of such use is in prediction of protein function. The characteristic of proteins, which allows them to function within an organism, is their ability to bind other molecules. They bind to other molecules similarly as jigsaw puzzle fit together, by matching their shape to the shape of target molecule. The function of unknown protein can therefore be estimated by comparing its shape to shapes of known proteins with known functions.

One of the traditional ways of solving the maximum common subgraph problem is by reduction to a maximum clique problem. The two input graphs, in which the maximum common subgraph is to be found, are multiplied to form a product graph, which is then input to the maximum clique algorithm. The result of the latter are used to identify the nodes of the input graphs that form the maximum common subgraph. Although the maximum clique problem can be solved by a modern branch-and-bound based algorithm for general graphs, such approach is far from optimal. Some special properties of the product graph can be exploited to guide the maximum clique search. Namely, the modern state-of-the-art clique search programs use coloring as auxiliary algorithm, but finding a good coloring of a graph itself a hard task.

In this article, we exploit the nature of the product graph to provide the maximum clique algorithm with a very good initial coloring or multiple such colorings. We perform experiments on a large database of small to medium sized graphs and demonstrate the efficiency of the proposed method against a state of the art method for solving maximum common subgraph problem.

Acknowledgments This work was funded by the Slovenian Research Agency (research core funding No. N2-0053) and by Hungarian National Research, Development and Innovation Office – NKFIH Fund No. SNN-117879.

Social Networks from Recommendation Graphs?

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A recommendation system is an information filtering system aiming at predicting the rating or preference a user would give to some items [1]. Nowadays recommendation engines provide us videos to watch, songs to listen, news to read and feed items to check in social network sites. Social recommendations utilize (1) the social relation data (e.g. friendship or geo-location data) and (2) contextual information based on user-item interactions (e.g. views, likes, comments, purchases). Many social experiments show that individuals are to some extent influence by others' behaviors, rather than making decision independently (in this context, decision can be, for example, watching the recommended video, or buying the recommended book) [2]. Social correlation theories, such as homophily and social influence, claims that user's preference is similar to or influenced by their socially connected friends. Analogous to the fact that users in the physical world are likely to seek suggestions from their friends before making a purchase decision and users' friends consistently provide good personalized recommendations, social relations can be potentially exploited to improve the performance of online recommendation systems.

For modeling social recommendation systems we use graphs; namely, a graph that represents the social (friendship, for instance) network of users, and a bipartite graph that represents the user-item interactions. According to these models, the following questions can be addressed:

- How the social network information can be used to obtain better recommendations?
- How to combine the so-called collaborative filtering method, which uses the user-item rating matrix, with information presents in the social network?
- Using one-mode projection methods for the bipartite network to the user side, can the social network be reconstructed with high precision?

The goal of the presentation is to give a brief overview of the main concepts of combining knowledge mined from social network together with collaborative filtering. In order to demonstrate our ideas we plan to use traces from real-world applications, which definitely give more experimental and theoretical insights to the ideas coming from the existing literature and from own developments as well.

Acknowledgment. The project has been supported by the European Union, co-financed by the European Social Fund (EFOP-3.6.3-VEKOP-16-2017-00002).

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An Integrated MILP Approach to Mobile Network Expansion in Presence of Subscriber Migration

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Worldwide telecommunications groups are both infrastructure operator and service provider. Hence, when planning the network expansion, these groups must consider the subscribers' dynamics, which they can influence through subsidies. Addressing both aspects together enables them to better optimize the network dimensioning, therefore avoiding unnecessary costs [1]. In this work, the network expansion represents the deployment and/or reinforcement of several technologies (e.g. 2G,3G,4G), assuming that subscribers to a given technology can be served by that technology or older ones. The objective of the resulting optimization problem is to minimize the punctual network expansion costs and subsidies, while being subject to both capacity and strategical constraints, such as minimum coverage and averaged debit performances. A Mixed-Integer Linear Programming (MILP) formulation is proposed to the solution of this optimization problem. The customer behavior in response to subsides is modeled through S-shape piece-wise linear functions which are linearized [2]. We assess numerically the resulting MILP formulation on realistic instances focusing on 3G/4G migrations. Our results show the scalability of the MILP model for 2 technologies and 100 sites. Moreover, they underline the cost-benefit in solving a unique optimization problem over the whole time-horizon (5 years) instead of decomposing the problem year by year, adding intermediary target objectives.

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MS 51: Mathematics of Biomedical Signal Processing

Adaptive Transformations in Biomedical Signal Processing

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Inspired by problems in ECG processing we have developed an adaptive transformation technique [2]. It is a variable projection method involving rational function systems. The main difference in our approach compared to the other transformation methods used in ECG processing is that instead of a fixed orthogonal or biorthogonal system we have a large pool of systems at hand. Then the system itself can be adjusted to the individual signal. As a result not only the coefficients of the orthogonal projection but also the system parameters carry information about the signal. The proper choice of the system parameters is a nonlinear optimization problem which depends on the specific problem. We have successfully used our idea for various problems in ECG signal processing including heartbeat modeling, and deriving medical parameters [2]. Moreover, the algorithms we have developed for ECG compression and heartbeat classification [4] outperform the other state of the art methods. The comparison tests were accomplished on the standard MIT-BIH Arrhythmia Database [1]. It is widely used as benchmark database for the validation of ECG processing methods. We note that our method can effectively be used for other types of signals as well. Such an example can be found where the problem of epileptic seizure detection in [3] EEG signals is considered.

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Using Unsupervised Diffusion Component Analysis on EEG of Posttraumatic Epilepsy Patients

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We have been developing and modifying analytic tools for human and animal data collected in the Epilepsy Bioinformatics Study for Antiepileptogenic Therapy (EpiBioS4Rx). The goal of the study is to identify relevant biomarkers of epileptogenesis after traumatic brain injury (TBI) and perform rigorous preclinical trials that will permit the future design and performance of economically feasible full-scale clinical trials of antiepileptogenic therapies. A fundamental challenge in discovering these biomarkers of epileptogenesis is that this process is likely multifactorial and crosses multiple modalities. Rather than considering one type of data, we must collect and analyze multi-modal data. The total amount of data collected in this study is unprecedented: video-electroencephalography (EEG) from scores of animals after TBI (using a fluid percussion model) recorded continuously for 6 months and prolonged continuous intensive care unit (ICU) EEG recordings from 300 humans in addition to MRI and blood data. We present results on EEG analysis, including scalp and depth EEG. Analyzing such a large dataset requires a powerful dimensionality reduction method with capabilities to remove noise from the EEG so that we can extract the underlying brain activity and use it to understand the development of epilepsy after TBI. We have developed Unsupervised Diffusion Component Analysis, previously used to study Alzheimer's disease using MRI data [1], and now more recently, on EEG data of TBI and posttraumatic epilepsy patients [2].

Acknowledgments This research was supported by the National Institute of Neurological Disorders and Stroke (NINDS) of the National Institutes of Health (NIH) under Award Number U54NS100064 (EpiBioS4Rx).

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Epileptic Seizure Detection via Hawkes Processes

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Epilepsy is the disease of unpredictability, affecting 1 % of the world's population. A novel technology under development is closed-loop neurostimulation, for the development of which a key component is the automatic interpretation and change detection of EEG signals collected on a portable device.

Standard features of an EEG signal for medical evaluation are high frequency oscillations (HFO) and inter-ictal discharges. Following the methodology developed in seismology a compressed representation of data is obtained by recording the events of interest only. Thus we get a point process, defined as a random sequence of points $T_0 = 0 < T_1 < T_2 \ldots$, and its associated a counting process $N_t = \#\{n \ : \ 0 < T_n \leq t\}$. Define its intensity as

$$\lambda_t := \lim_{\Delta \downarrow 0} \frac{1}{\Delta} \mathrm{E}\left[\mathrm{N}[\mathrm{t}, \mathrm{t}+\Delta) \mid \mathcal{F}_\mathrm{t}\right] \quad \text{a.s.}$$

where $\mathcal{F}_t$ is the history of $(N_s, s \leq t)$. Physiological considerations induce us to assume a certain feedback effect, hence the current intensity is assumed to be obtained as

$$\lambda_t = \mu + \int_{-\infty}^{t} g(t-u) dN_u, \qquad g(t) \geq 0, \tag{7}$$

with some $\mu > 0$ and a non-negative impulse response $g(u)$, see [1]. Special attention has been paid to exponential response functions, say $g(t) = \sigma e^{at}$ with $a < -\sigma < 0$, see [2].

Considering a parametric family of Hawkes processes the maximum-likelihood estimator of the unknown parameter will be studied, revisiting [2]. Extensive computational results will be presented based on both real and simulated data, establishing physiologicaly relevant regions of the parameter space. In addition, a close connections with the theory of system identification for linear stochastic systems (LSS), will be established. Finally, we demonstrate the applicability of our results for real time change detection, and possible extension for multivariate Hawkes processes will be discussed, see [3].

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MS 52: Graphisoft

Architectural Applications of the Straight Skeleton

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The *straight skeleton* (or *angular bisector network, ABN*) of a planar polygon is first defined by Aichholzer et. al. [1]. Solely made up of straight line segments, it can serve as a simpler alternative for skeletal structures (such as the medial axis) in many applications. Its algorithmic definition is also appealing as it makes computer implementations seemingly straightforward.

The ARCHICAD architectural modeling software uses straight skeletons to create the 3D model of multi-plane roofs (above a closed chain of straight walls), and of slabs with slanted sides. Generalizations of the straight skeleton – and thus extensions of the generation algorithm – are needed to meet the demands of roof modeling in architecture. For example vertical and outward-pitched roof facets and holes in the base polygon are common in architectural practice. These challange the implementor on both the theoretical and the technical sides.

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Self-Adaptive Nonlinear Least Square Optimization for Geometric Calculations

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Three dimensional architectural structures are often constructed by sweeping a set of 2D shapes —profile—. Proper parameterization to control the shape and size of the profile geometry provides significantly more flexible design environment for the architect.
Recent development project at GRAPHISOFT was aimed to provide Parametric Profile functionality. Edge-offset was selected to be the basic shape and size change operation. A new geometry-calculation engine has been developed, which is responsible to solve the problem arising from the combination of edge-offset operations and user defined constraints. The solution is achieved by minimizing sum of squared residuals [1]. In order to achieve super fast response times —a must for interactive editing— the solution process takes advantage of the sparsity of involved matrices. Most importantly, the problem-formulation uses **Homotopy Continuation** [2] technique in novel way. Automatic control of the continuation parameter is achieved via an auxiliary residual, embedded into the optimization process. This way the control becomes **self-adaptive**; capable to adjust to the characteristics of the actual problem in hand: For easy problems it may quickly escape unnecessary continuation "steps", while for hard-to-solve problems it ensures proper convergence via Homotopy Continuation. Though such optimization-embedded Continuation technique may slightly impact convergence speed, it provides superior solution stability.

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Boolean Operations Between Polyhedric Solids in ArchiCAD

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Workflow of our architectural design software — ARCHICAD — relies heavily on boolean operations between polyhedral solids represented in BREP format.

The boolean operation is implemented with a fallback system: first a fast but not robust algorithm tries to solve the problem, in case of its failure a slower but much more robust algorithm works.

Former is an implementation of Martti Mäntylä's work [1] which has known limitations in handling of non-2-manifold boundary parts of polyhedra and has problems with numerical inaccuracies. Both problems arise sometimes while transforming even simple architectural models to 3D polyhedral model.

To meet these demands GRAPHISOFT developed the latter algorithm of the fallback chain which is called EWT (Exact With Triangles). This algorithm uses exact arithmetic on rational numbers instead of the traditional floating-point arithmetic. By this and by triangulating the boundary surface of the polyhedra it successfully eliminates topological problems arising from numerical inaccuracy. Non-2-manifold parts of the polyhedra are handled correctly.

Concerning speed, EWT falls behind Mäntylä's algorithm. Effort has been made to improve speed by subsidiary floating-point arithmetic calculations and error-estimation, which filters calculations made in exact arithmetic.

Keywords: Boolean Operations on Polyhedra; BREP; 2-manifold boundary; Arbitrary-precision Arithmetic

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Constrained Delaunay Triangulation

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The following problems will be discussed. Let n be the number of points given on the plane. We are looking for triangles whose vertices fit the specified points, and no given point lies inside the circumcircle of any triangle. This is the well-known Delaunay triangulation [1]. The same points are given. Each given point belongs to a specified region, where all points of the region are closer to that given point than to any other. This is called the Voronoi diagram [2]. There is a duality between Voronoi diagram and Delaunay triangulation, each one is easily obtained from the other: if we connect the points of neighboring regions; thus, we get the Delaunay triangulation. Since we want to generate 3D terrain model, therefore a border should be given, and the points are placed inside, this triangulation should be solved. The border polygon may have holes. Sectors or lines can be added, and they should be the side of a triangle [3]. The final result will be triangles in 3D, because the given points were also in 3D, but in triangulation only x and y values are used. Finally, a small part of the implementation will be examined [4]. We also draw attention to possible problems.

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MS 53: Morgan Stanley

Quantitative Finance – the Beauty and the Beast

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Understanding and predicting the financial world is an exciting and challenging endeavor. Financial markets together with their sophisticated products, the pertaining rules, and the participants' preferences and beliefs change from one moment to the next. This creates an evolving, complex ecosystem with quite fundamental differences from other disciplines in Natural Sciences. Given the complexity, non-stationarity and transitivity most of the quantitative financial models are phenomenological. They simplify reality and only work well in a rather narrow domain of applicability in the space of market parameters and time. The talk will revolve around questions like what is the goal of a financial model, when is it good and when is it wrong? What can the model predict about the future of the markets? How can the financial players use these models for their advantage and how can they lose fortunes when they are inappropriate? How do they face the Beauty and the Beast?

A Least-Square Method to Calculate Counterparty Exposure

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In this talk we recite the results of Longstaff and Schwartz [1] to use a least-squares Monte Carlo method to price American options. We then discuss the problem of calculating a Firm's credit exposure to its trading counterparties, and present how the same method can be tailored for this purpose, as published by Kan, Frank, Mozgin, Reesor [2].

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How much should you trust your Least Squares Method as a risk manager?

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In a Monte Carlo framework the least squares method (LSM) is a widely used and very efficient approximation technique when one would like to compute the value of an early exercise option for pricing, or future exposures in a counterparty risk setting. In the latter we are not only interested in calculating the expectation of future exposures (i.e. Expected Positive Exposure (EPE)), for risk management purposes we also heavily rely on quantiles (i.e. Potential Future Exposure (PFE)) of the distribution. In this paper we compare the future exposure distribution of equity options calculated by the LSM to alternatives. We consider the novel stochastic grid bundling method (SGBM) and analytical solutions if available, and investigate the exposure metric (EPE, PFE) differences between the methods for selected option maturities and moneyness levels.

Credit Default Risk and Correlated Defaults

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We briefly present a multi-factor Gaussian copula portfolio model for default risk. The model assumes three types of systematic factors driving the asset value of each company. These factors represent the state of the global economy and the economic conditions of different geographical regions and industries. The corresponding factor loadings play a key role in the model, as they capture the correlation structure between the asset returns of different companies and therefore influence the joint probabilities of default. Higher correlation between the asset returns of different companies in a portfolio increases the likelihood that multiple companies will default simultaneously, thus increasing the likelihood of extreme losses in the portfolio. Hence, accurately measuring these correlations is essential for the identification of portfolio risk. We describe a possible methodology for measuring the correlations between asset returns of different companies, which can be used for calibrating the corresponding factor loadings. The approach relies upon single-name CDS spread data. We will also analyze of the structure of correlations obtained using this methodology.

Contributed talks

Inverse Problems in Industry: Theory and Methods

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Inverse problems arise in a number of important practical applications, ranging from biomedical imaging to seismic prospecting. This work sheds light on both the underlying mathematics and the computational methods used to solve inverse problems. It also addresses specialized topics like image reconstruction, parameter identification, total variation methods, nonnegativity constraints, maximum likelihood estimation, Bayesian estimation and regularization parameter selection methods.

Physical theories allow us to make predictions: given a complete description of a physical system, we can predict the outcome of some measurements. This problem of predicting the result of measurements is called the forward problem. The inverse problem consists of using the actual result of some measurements to infer the values of the parameters that characterize the system. While the forward problem has (in deterministic physics) a unique solution, the inverse problem does not. As an example, consider measurements of the gravity field around a planet: given the distribution of mass inside the planet, we can uniquely predict the values of the gravity field around the planet (forward problem), but there are different distributions of mass that give exactly the same gravity field in the space outside the planet. Therefore, the inverse problem — of inferring the mass distribution from observations of the gravity field — has multiple solutions.

A collection of MATLAB m-files used to generate many of the examples and figures are available in this work. These resources enable scholars to conduct their own computational experiments in order to gain insight. Finally, we provide templates for the implementation of regularization methods and numerical solution techniques for industrial inverse problems like the determination of the depth dependence of the director field in a liquid crystal cell from polarized light measurements [1], capacitance tomography for monitoring flow in pipes [3], and a problem in which the ocean current is estimated from the position of a cable towed behind a geophysical survey ship [2].

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Queues with Choice from a Symmetry Perspective

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Recently, a queueing model where in customers are given an opportunity to choose between two queues was introduced [4]. The queue length information provided to the customers is not up-to-date. Instead, customers were given the queue length some time units in the past. This time delay impacts the dynamical behavior of the queues and hence the decision-making process of the customers. We revisit this queues-with-choice model from a symmetry perspective [3]. We show, using similar techniques used in [1, 2], that the symmetric structure of the model can be used to classify the types and kinds of solutions that can occur. In particular, our results explain why only asynchronous periodic solutions and symmetric equilibrium solutions arise in such model, while synchronous periodic solutions and asymmetric equilibrium solutions do not occur. These additional insights on the dynamical behavior of queues will help companies to be more aware of the consequences of providing delayed queue length information to their customers.

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Numerical Computation of Electromagnetic Fields in 3D Axisymmetric Singular Domain

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We propose a new variational method to compute 3D Maxwell's equations in an axisymmetric singular 3D domain, generated by the rotation of a singular polygon around one of its sides, namely containing reentrant corner or edges. We consider the equations written in (r, θ, z) and use a Fourier transform in θ to reduce 3D Maxwell's equations to a series of 2D Maxwell's equations, depending on the Fourier variable k. The principle is to compute the 3D solution by solving several 2D problems, each one depending on k.

Let us denote by $(\mathbf{E}_k, \mathbf{B}_k)$ the electromagnetic field for each mode k. Following [1] and [2], it can be proved that this solution can be decomposed into a regular and a singular part. The regular part can be computed with a classical finite element method. The singular part is more difficult to compute: it belongs to a finite-dimensional subspace. Its dimension is equal to the number of reentrant corners and edges of the 2D polygon that generates the 3D domain.

We will first consider the computation of $\mathbf{x}_k^s$ and $\mathbf{y}_k^s$, the singular part of the electric and magnetic field. We will then derive the non stationary variational formulation to compute the total part of the solution. Following [2], this will require first to derive the system of equations solved by the singular parts for each k. Then to derive and solve the time-dependent variational formulation depending on k, for each mode. Finally to reconstruct the approximate 3D electromagnetic fields from each mode k. Numerical examples to illustrate our method will be shown.

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A Reduced 3D Model of a Passive Admixture Transport in Shallow and Slightly Curved Natural Watercourse

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Some further results of research [1] are presented. Main goal of the study is to provide a simplified 3D mathematical model for admixture spreading process in shallow shear flows and to testing it. This model is oriented to the hydrological and ecological problems, so it can be applied to natural streams like rivers and channels.

The distinctive feature of such watercourses is a considerable difference in sizes of their length, width and depth. For example, the ratio between the characteristic depth and width for a typical lowland river varies from 1:10 to 1:200.

The formulation of the problem is as follow. A passive admixture spreads in an open turbulent flow of incompressible viscous fluid in some section of river or channel. The river-bed is assumed known and slightly curved. Also the stream is assumed lengthy and shallow. So, the geometry of the considered part of the stream can be described by known functions smooth enough.

The passivity of admixture means that the mathematical description of the process splits into two subsystems of equations. The first one – the hydrodynamic subsystem – allows to find the velocity field in fluid, and the second one – the concentration subsystem – allows finding the concentration of admixture in the stream with known velocity field.

The reduced 3D model takes into account the cross-structure of a stream. This is a strong particular feature of the proposed model. That allows us to study the admixture spreading in a channel with varying width and depth more accurate than by utilizing the on-depth averaged models. For example, we can catch the phenomenon of occurrence the opposite flow in a near-surface region, which may be caused e.g. by means of the wind action.

The numerical results show that this reduced 3D model adequately describes the spreading processes in natural streams. It provides acceptable accuracy and allows the improvements by means of applying the recurrent correction procedure.

Acknowledgments The research is partly supported by a grant from the Vladimir Potanin Charity Fund (project GPK-96/17). The results of the study will be used in the Master Program "Computational Mechanics and Information Technologies".

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New Special Functions and Integral Transforms

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Special functions are the back bone of mathematical physics. They are the most appropriate tool to deal with analytical and numerical solutions of linear and non linear ordinary and partial differential equations.

The advent of modern computers and of symbolic calculus rather than making this branch of mathematics obsolete has determined further interest in the underlying "calculus" and generalized forms.

We develop a new point of view to introduce families of functions, which can be identified as generalization of the ordinary trigonometric or hyperbolic functions [1]. They are defined using a precedure based on umbral methods, inspired to the Bessel Calculus of Bochner, Cholewinsky and Haimo [2]. We propose further extension of the method and of the relevant concepts as well and obtain new families of integral transform allowing the framing of the previous concepts within the framework of generalized Borel transforms.
We establish a link with umbral methods and provide examples of the relevant applications for the solution of problems of wave propagation.

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Optimal Control of Heavy Metals Phytoremediation

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Heavy metals enter aquatic systems as a result of very different human activities involving the mining, processing and use of substances containing metal pollutants. Phytoremediation is a cost-effective plant-based approach of remediation for heavy metal-contaminated bodies of water, that takes advantage of the ability of algae to concentrate elements from the environment, metabolizing them in their tissues.

This paper deals with the optimization of different issues related to phytoremediation methods, by combining mathematical modelling, optimal control of partial differential equations and numerical optimization [1, 2, 3]. In particular, we propose a 2D mathematical model bringing together the system for shallow water hydrodynamics and the system of coupled equations modelling the concentrations of heavy metals, algae and nutrients in large waterbodies. We also present a full algorithm for computing the numerical solution of the system.

We are interested in determining the minimal quantity of algae to be used, and also in locating the optimal place for such algae mass. These questions are formulated as optimal control problems for this scenario, and several numerical results for a realistic problem are presented.

Acknowledgments The authors thank the funding from project MTM2015-65570-P of MINECO/FEDER (Spain). The help and support provided by DHI with the MIKE21 modelling system is also deeply appreciated.

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DRBEM Solution of Mhd Flow in an Array of Electromagnetically Coupled Rectangular Ducts

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This work presents the dual reciprocity boundary element method (DRBEM) solution to magnetohydrodynamic (MHD) flow of an electrically conducting fluid in a single and two parallel ducts which are separated by conducting walls of arbitrary thickness in the direction of external magnetic field. The no-slip velocity condition is imposed on the duct walls, and outer sides of all the walls are electrically insulated. The DRBEM discretizes the MHD convection-diffusion equations in the ducts and the Laplace equations on the interconnected walls as a whole by using constant boundary elements. It makes enable to impose the coupled wall conditions of the induced magnetic fields and their normal derivatives, on the passages from the conducting walls to the fluid, while solving MHD equations of the fluid coupled with the conductivity equations of the walls. The effects of the wall thickness and strength of the applied magnetic field are studied on the flow and induced magnetic fields. It is shown that, the conducting walls in the double ducts have a strong influence on the currents near the walls and the core flow increases on the co-flow case but there is a strong reduction in the core flow in the counter-flow case. As Hartmann number increases flow is concentrated in front of the sides walls in terms of two loops, and side layers are developed for the flow in single and double ducts. The coupling between the ducts with conducting thick walls induce reversed flow and counter current flows which may be used for the heat and mass transfer in fusion applications. The proposed numerical scheme using DRBEM captures the well-known MHD flow characteristics when Hartmann number increases.

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Solution of MHD Flow with BEM Using Direct Radial Basis Function Interpolation

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Magnetohydrodynamics (MHD) focuses on the flow of electrically conducting fluid in the presence of an external magnetic field which has important industrial applications such as MHD pumps, liquid metal productions, nuclear reactors and blood flow measurements. In this study, the two-dimensional steady MHD Stokes and MHD incompressible flows of a viscous and electrically conducting fluid are considered in a lid-driven cavity under the impact of a uniform horizontal magnetic field. The governing equations are the Navier-Stokes equations of hydrodynamics coupled with Maxwell's equations of electromagnetics through Ohm's law neglecting the convective terms due to the small values of Reynolds number (Re) in the MHD Stokes flow case [1, 2]. The MHD equations are solved iteratively in terms of velocity components, stream function, the vorticity and pressure by using direct interpolation boundary element method (DIBEM). In DIBEM [3], all the terms except the Laplacian are treated as inhomogeneity and fundamental solution of the Laplace equation is used to convert the domain integrals to boundary integrals using Green's theorem. The complete kernel of the domain integral composed of the product of the fundamental solution and inhomogeneity term is directly interpolated by using radial basis functions which is the main difference from the dual reciprocity boundary element method (DRBEM). The boundary is discretized by constant elements and the sufficient number of interior points are taken. The interpolation points are different from the source points due to the singularities of the fundamental solution. The numerical results are obtained for several values of Hartmann number (M) to analyze the effect of the magnetic field on both the Stokes and incompressible flows. It is found that as Hartmann number increases, the main vortex of the flow shifts through the moving top lid with a decreasing magnitude and secondary flow below it is squeezed through the main flow leaving the rest of the cavity almost stagnant. Vorticity circulates in the cavity when Re increases. The increase in M develops side layer near the moving lid, but weakens the effect of increase in Re in the MHD incompressible flow.

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Properties of Local Defect Correction for Boundary Element Methods

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The local defect correction is a technique for obtaining the numerical solution of a partial differential equation on a composite grid without directly solving on the grid. The approach is to use the solution on a fine grid, which is only in a small part of the domain where the solution changes rapidly, to compute the defect of the system on a global coarse grid. This technique has been well studied in other methods like the finite difference method. In the Boundary Element Method (BEM), only the boundary of the domain is discretised. This is a big advantage over the Finite Element Method (FEM). However, BEM matrices are full matrices compared to FEM which has sparse matrices. Thus, the BEM would benefit a lot from such a technique since using fine grids to capture rapid activity of the unknowns would result in bulky matrices. The ideas used to develop the local defect correction algorithm in finite difference methods can be expanded to develop a similar algorithm for the boundary element method. However, the comparison is not direct given that in the boundary element method, the solution is computed by integrating over the global boundary. We have proposed an algorithm which we showed that it works for the boundary element method. In the present work, we develop convergence properties for that algorithm. We formulate the algorithm as a fixed point algorithm and study the spectral properties of the iteration matrix. The results show that for a Neumann problem, we can always expect convergence. Having also shown that it is cheaper than solving directly on a global fine uniform grid or composite grid, the algorithm then presents a real alternative for application in the boundary element method for problems with localised regions of high activity.

Acknowledgments The authors are grateful to Swedish SIDA Phase IV bilateral support to Makerere University 2015 - 2020, Project 316, for their support in this work.

Application of Splitting Algorithm for Solving Advection-Diffusion Equation on a Sphere

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A numerical algorithm for the solution of advection-diffusion equation (ADE) on the surface of a sphere is suggested. The velocity field on the sphere is assumed to be known and non-divergent. The surface of sphere is partitioned into non-overlapping grid cells of trapezoidal shape plus two round pole cells centered at the North and South poles. The discretization of ADE in space is carried out with the help of the finite volume method, and the Gauss theorem is applied to each grid cell. For the discretization in time, the symmetrized double-cycle componentwise splitting method and the Crank-Nicolson scheme are used [1]. The numerical scheme is of second order approximation in space and time, correctly describes the balance of the mass of substance in the forced and dissipative discrete system, and is unconditionally stable. In the absence of external forcing and dissipation, the total mass and L_2-norm of solution of discrete system are conserved in time [2].

The one-dimensional periodic problems arising at splitting in the longitudinal direction are solved with Sherman-Morrison's formula [3] and Thomas's algorithm [4]. The one-dimensional periodic problems arising at splitting in the latitudinal direction are solved by the bordering method that requires a prior determination of the solution at the poles. The resulting linear systems have tridiagonal matrices and are solved by Thomas's algorithm. Parallel processors can be used for solving the split problems. The suggested implicit method is direct (without iterations) and rapid in realization. It can also be applied to linear and nonlinear diffusion problems, some elliptic problems and adjoint advection-diffusion problems on a sphere.

The new algorithm is tested with various advection-diffusion problems. The results show high accuracy and efficiency of the method.

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The Effect of Welding on the One-Dimensional Cutting-Stock Problem: The Case of Fixed Firefighting Systems in the Construction Industry

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Safety is paramount in the construction industry and the fixed sprinkler and water spray systems used in firefighting involve networks of pipes of various lengths. Manufacturers of fixed firefighting systems need to either cut the existing stocks to length —a (one-dimensional) cutting-stock problem— or lengthen the existing stocks or leftover segments through welding —a (one-dimensional) cutting-stock problem with welding. Safety requirements allow only one weld per length of pipe.

The real case of a Hungarian manufacturer of fixed firefighting systems informs this presentation, which argues that the cutting-stock problem with welding (with single- or multiple-size stocks) may be converted to an equivalent cutting-stock problem (with multiple-size stocks). Readily available algorithms and softwares may then be used to generate an optimal cutting plan for the equivalent cutting-stock problem. Subject to certain restrictions, the optimal cutting plan for the equivalent cutting-stock problem may then be converted to cutting patterns for the original cutting-stock problem with welding.

The Inverse Problem Approach for x-ray Radiographic Tomography

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X-ray radiographic tomography has many applications in industry, medical treatment and nuclear physics. From a radiograph, which records the attenuation of x-ray intensity, to reconstruct an object physical parameters is an inverse problem. In this talk, the ill-posedness of the inverse problem will be analyzed, and the proposed mathematical model and numerical algorithm will be introduced. Numerical tests will be given to illustrate the efficiency of the new method. Different from the traditional reconstruction methods, such as the Fourier domain interpolation method and the Filtered back projection method, we introduce the variational method to reconstruct the axially symmetric objects transmitted by fan beam x-rays. The proposed method has advantage on tackling the blurred and noisy projection data. It also improves the image reconstruction detail and quality. Meanwhile the computational cost reduction can be achieved.

Acknowledgments The research is partially supported by National Natural Science Foundation of China (grant 11571003).

Moment Matching Based Model Reduction for Quadratic-Bilinear Descriptor Systems

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In the model order reduction of (partial) differential-algebraic equations the treatment of nonlinearities is an open field of research. We approach the nonlinearities by introducing additional variables and transforming the equations into an equivalent quadratic-bilinear system for which we investigate two methods of moment matching based model order reduction. On the one hand we consider multimoment matching regarding the multivariable higher order transfer functions of the quadratic-bilinear system. On the other hand we apply the technique of the associated transform on the transfer functions, yielding a univariable transfer function. For the associated linear system the well-studied methods of linear moment matching can be applied to deduce a reduced model. We compare the performance of two approaches with regard to accuracy, efficiency and need of memory.

Thermoviscoelastic Kelvin-Voigt Model

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Let $\Omega \subset \mathbb{R}^n$, $n = 2, 3$. We consider the following initial boundary value problem

$$\frac{\partial v}{\partial t} + \sum_{i=1}^{n} v_i \frac{\partial v}{\partial x_i} - 2\mathrm{Div}(\nu(\theta)\mathcal{E}(v)) - \varkappa \frac{\partial \Delta v}{\partial t} - 2\varkappa \mathrm{Div}\big(v_i \frac{\partial \mathcal{E}(v)}{\partial x_i}\big) + \nabla p = f, \quad (t,x) \in Q_T;$$

$$\mathrm{div}\ v = 0, \quad (t,x) \in Q_T; \qquad v|_{t=0} = v_0, \quad x \in \Omega; \qquad v|_{[0,T]\times\partial\Omega} = 0;$$

$$\frac{\partial \theta}{\partial t} + \sum_{i=1}^{n} v_i \frac{\partial \theta}{\partial x_i} - \chi \Delta\, \theta = 2\nu(\theta)\mathcal{E}(v) : \mathcal{E}(v) + 2\varkappa \frac{\partial \mathcal{E}(v)}{\partial t} : \mathcal{E}(v) + g, \quad (t,x) \in Q_T;$$

$$\theta|_{t=0} = \theta_0, \quad x \in \Omega; \qquad \theta|_{[0,T]\times\partial\Omega} = 0.$$

Here $v(x,t) = (v_1, ..., v_n)$ is the velocity vector-function, $\theta(t,x)$ is the temperature function, $p(x,t)$ is the fluid pressure, $f(x,t)$ is the density of external forces, g is the external heat source, $\mathcal{E}(v) = (\mathcal{E}_{ij}(v))_{j=1,...,n}^{i=1,...,n}$, $\mathcal{E}_{ij}(v) = \frac{1}{2}(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i})$ is the strain velocity tensor, $\chi > 0$ is the coefficient of thermal conductivity, $\varkappa > 0$ is the time of retardation (delay), $\mu_0 > 0$ is the initial viscosity of a fluid, $\mu(s)$ is the viscosity of a fluid and $\widetilde{\mu}(s) = \mu_0(s) + \mu(s)$.

This initial-boundary value problem under consideration describes the weakly concentrated water polymer solutions motion. This mathematical model also is called Kelvin-Voigt model. Also in this mathematical model the viscosity depends on a temperature, which leads to emergence of additional heat balance equation (it is a parabolic equation with nonsmooth coefficients and with right part from $L_1(0,T;L_1(\Omega))$. For the initial-boundary value problem under consideration the existence theorem of weak solutions is proved. For this the topological approximation approach for hydrodynamic problems is used.

Acknowledgments This research was supported by the Ministry of Education and Science of the Russian Federation (grant 14.Z50.31.0037).

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Problem of Viscoelastic Media with Memory Motion

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Integrating the Jeffreys-Oldroyd rheological relation $(1+\lambda\frac{d}{dt})\sigma = 2\nu(1+\varkappa\nu^{-1}\frac{d}{dt})\mathcal{E}$ (where $\frac{d}{dt}=\frac{\partial}{\partial t}+\sum\limits_{i=1}^{n} v_i\frac{\partial}{\partial x_i}$, $\mathcal{E}=\{\mathcal{E}_{ij}\}_{i,j=1}^{n}$, $\mathcal{E}_{ij}=\frac{1}{2}(\frac{\partial v_i}{\partial x_j}+\frac{\partial v_j}{\partial x_i})$ is the strain rate tensor and $\lambda,\varkappa,\nu$ are positive constants) along velocity field v, expressing σ from this relationship and substituting it in the general equation of fluid motion we get the following initial-boundary value problem

$$\frac{\partial v}{\partial t}+\sum_{i=1}^{n} v_i\frac{\partial v}{\partial x_i}-\mu_0\Delta v-\mu_1\mathrm{Div}\int_0^t \exp\left(\frac{s-t}{\lambda}\right)\mathcal{E}(v)\,(s,z(s;t,x))\,ds+\nabla p=f; \tag{8}$$

$$\operatorname{div} v(t,x)=0,\quad (t,x)\in Q_T; \tag{9}$$

$$z(\tau;t,x)=x+\int_t^\tau v\,(s,z(s;t,x))\;ds,\quad 0\leqslant t,\tau\leqslant T,\quad x\in\overline{\Omega}; \tag{10}$$

$$v(0,x)=v_0(x),\ x\in\Omega;\quad v(t,x)=0,\quad (t,x)\in[0,T]\times\partial\Omega. \tag{11}$$

Here the integral term in (8) takes into account the memory of the system. For simplicity, we assume $\rho=1$ in rheological relation and $\mu_0=2\varkappa$, $\mu_1=2(\nu-\varkappa)$.

Theorem 1. Let $f=f_1+f_2$, where $f_1\in L_1(0,T;H)$, $f_2\in L_2(0,T;V^{-1})$ and $v_0\in H$. Then there exists a weak solution of problem (8)-(11).

Motion model with memory on infinite time interval

Let $Q=(-\infty,T]\times\Omega$, where $T>0$, $\Omega\subset\mathbb{R}^n$, $n=2,3$, is a bounded domain with boundary $\partial\Omega\subset C^2$. We consider in Q the problem

$$\frac{\partial v}{\partial t}+\sum_{i=1}^{n} v_i\frac{\partial v}{\partial x_i}-\mu_0\Delta v-\mu_1\mathrm{Div}\int_{-\infty}^t \exp\left(\frac{s-t}{\lambda}\right)\mathcal{E}(v)(s,z(s;t,x))ds+\nabla p=f; \tag{12}$$

$$\operatorname{div} v(t,x)=0,\quad (t,x)\in Q;\quad v(t,x)=0,\quad (t,x)\in(-\infty,T]\times\partial\Omega; \tag{13}$$

$$z(\tau;t,x)=x+\int_t^\tau v(s,z(s;t,x))\,ds,\quad t,\tau\in(-\infty,T],x\in\overline{\Omega}. \tag{14}$$

Theorem 2. Let $f\in L_2(-\infty,T;V^{-1})$. Then problem (12)-(14) has at least one weak solution.

Problems with memory along trajectories on the half-line $(-\infty,T]$ occur for many models of viscoelastic fluids motion, but existence theorems for these problems for infinite intervals $(-\infty,T]$ are unknown for us.

Acknowledgments This research was supported by the Ministry of Education and Science of the Russian Federation (Grant 14.Z50.31.0037).

Optimal Feedback Control Problem for Bingham Fluid Motion

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The problem of control (optimal control) of fluid motion by external forces often arises in practical applications. Usually when dealing with such problems, the control is chosen from some given (finite) set. However, in papers of V.G. Zvyagin, V.V. Obukhovskii, M.V. Turbin (see, for example, [1, 2] and the bibliography therein) it were considered problems with external forces (control), depending on the velocity of the fluid (such problems are called problems with feedback). This approach allows to select the control more precisely, since in this case the control is chosen not from the finite set of available controls, but belongs to the image of some multivalued map (naturally, this map satisfies to some conditions, namely, it must be bounded, upper semicontinuous, weakly closed and has non-empty, compact and convex values). The solution of control problem for considered fluid model is the pair (v, f), where v is the velocity of the fluid, and f is the control (density of external forces). Moreover, f belongs to the image of some multivalued map depending on the velocity v of the fluid. In connection with the fact that there can be many such pairs, it naturally arises the concept of an optimal solution. This solution gives a minimum to a given quality functional.

In this talk we consider the feedback control problem for the mathematical Bingham model of fluid motion in the three-dimensional case with periodic conditions on spatial variables. First it is shown that there exists a solution to the control problem with feedback. Then it is proved that among the solutions of the considered problem there exists a solution giving a minimum to a given quality functional.

Acknowledgments This research was supported by the Ministry of Education and Science of the Russian Federation (grant 14.Z50.31.0037).

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Solid-Fluid Coupling in a Fully Lagrangian Framework

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The simulation of multiphase flows including granular and fluid phases is of great interest in a wide variety of industrial applications, such as chemical process engineering, design of conveyor systems or abrasion modeling. In this context, the granular phase is often described by the discrete element method, which calculates the trajectory of each individual solid particle in a Lagrangian manner while resolving inter-particle and geometry collisions. While the models behind individual interactions are generally not very complex, the necessary data structures and neighborhood algorithms often have a major impact on performance. Here, we present the coupling of this approach to an existing Lagrangian generalized finite difference method for the fluid phase. Our method, called finite pointset method, is developed at Fraunhofer ITWM and has been successfully used in a wide variety of practical applications [1, 2, 3]. Coupling these two approaches enables us to treat all phases in a common framework and to use the existing efficient and scalable data structures and algorithms, while also benefiting from the advantages of meshfree fluid solvers in free surface problems or rapidly changing flow geometries. We will validate our scheme and present simulation results for a water turbine with sand particles immersed in the fluid phase. In this application, the granules may have non-negligible sizes relative to the geometry which motivates a two-way coupling and resolution of individual interactions. We can further make use of the advantages of meshfree methods in handling moving geometries.

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Double Freeform Surfaces Design for Laser Beam Shaping: A Least-Squares Approach

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Freeform optics concerns the construction and/or computation of optical surfaces that convert a given source distribution of light into a desired target distribution. In this contribution we discuss freeform optics for laser beam shaping.

The problem we investigate is the following. Given a source $\mathcal{S}$ emitting a parallel beam of laser light and two separated lenses with altogether two freeform surfaces, determine the shape of these surfaces such that after two refractions the laser beam is still parallel and hits a target screen $\mathcal{T}$ with a desired desired illuminance. From the principle of equal optical path, we can derive a relation of the form

$$u_1(\boldsymbol{x}) + u_2(\boldsymbol{y}) = c(\boldsymbol{x}, \boldsymbol{y}),$$

where $u_1(\boldsymbol{x})\,(\boldsymbol{x} \in \mathcal{S})$ and $u_2(\boldsymbol{y})\,(\boldsymbol{y} \in \mathcal{T})$ define the location and shape of the two freeform surfaces, and where $c(\boldsymbol{x}, \boldsymbol{y})$ is a non-quadratic cost function. From this relation we can determine the optical map $\boldsymbol{m} : \mathcal{S} \to \mathcal{T}$. Combined with energy conservation, this relation gives rise to a Monge-Ampère equation (MAE) with transport boundary conditions.

For the standard MAE with quadratic cost function we have developed a least-squares method [1]. We have extended this method for a MAE with non-quadratic cost function describing a freeform lens [2]. We employ the latter method for our laser beam shaping problem. Both least-squares methods are two-stage procedures. First, we compute the optical map in a least-squares sense from a constrained minimisation problem for the energy balance, and second, we compute the shape of the freeform surfaces from the mapping.

Our algorithm is efficient and can handle very complicated target distributions. The performance of the method is shown for several problems, for example, the design of an optical system that converts a top-hat distribution into a Gaussian. We can also handle non-rotational symmetric distributions.

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Damage Detection in Thin Plates via Time-Harmonic Infrared Thermography

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Non-destructive damage detection has become a very active research topic recently. In all material there are micro-defects such as voids and cracks that can reach a critical size supposing the total collapse of the structure after undergoing several stress-relaxation cycles. In order to prevent the failure during the operation manufacturers set periodic tests. These tests aim to detect the cracks when they have grown enough to be detectable but before they suppose a risk. Given that the actual non-destructive tests are very slow there is a great interest in looking for faster, cheaper and more robust methods.

In this paper we study a promising new method consisting on heating the plate to be inspected with some kind of lamp and trying to detect the position number and size of the defects from a thermogram of one side of the plate. Finding the set of cracks that give raise to a given temperature distribution is an ill posed non-linear inverse problem which is regularized and stated as a minimization problem. In order to solve this problem the topological derivative [1] will be used. This is a fairly new method which gives an estimator of the number, size and position of the cracks with no need for iteration or a priori knowledge. It has already been used in a two dimensional thermal propagation problem in an unbounded media in [2] with very good results. It also has being proved to work in finite two-dimensional plates with promising results in the steady-state situation [3]. We will show how to improve the reconstructions by suitably combining monochromatic time-harmonic results in the spirit of [4].

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Approximating a Class of Non-Linear Third-Order Ordinary Differential Problems

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Third-order differential equations are important for various applications in the sciences and in engineering, see *e.g.* [1, 2] and the references therein. In this work we consider the matrix case and develop a numerical scheme by using matrix splines to find the solutions of the following non-linear differential problem

$$Y'''(x) = f(x, Y), \quad Y \in \mathbb{R}^{n\times n}, \quad x \in [a, b].$$

Certainly higher-order ordinary differential equations can always be reduced to a first-order system of ordinary differential equations, and subsequently standard methods can be exploited to obtain numerical estimates. This conventional approach, however, comes with an undesirable increase in computational cost. Our method avoids this problem. In recent years, direct integration methods have attracted considerable attention and for other higher-order cases we have already demonstrated appreciable improvements in speed and accuracy, see [3, 4, 5]. After an outline of the third-order algorithm, we also present some instructive examples of the method.

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Motion of Spherical Particle Attached to the Interface Between Two Viscous Fluids

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The calculation of drag force of particles, which move at the interfaces between two viscous fluids, is of crucial importance for the characterization of 2D ordering and diffusivity of inclusions at material interfaces and bio-membranes. The obtained results are a tool for modeling of the complex multi-particle interaction problems in construction of antireflective surface coating of solar panels, micro-lens structures in CCD technologies, 2D ordering of protein molecules and bio-memory chips.

The problem was solved semi-analytically using the Mahler-Fox transformation for water/air interface and three phase contact angles smaller than 90° [1]. We propose a numerical method for the calculation of the drag force coefficient based on the gauge formulation of the Stokes equations for two viscous fluids valid for all values of the contact angles [2]. The weak singularity of solutions at the contact line is studied using an appropriate asymptotic method. The isolation of the type of singularity helps us to construct an efficient second order numerical scheme based on the ADI approach. The problem is solved numerically for a wide range of positions of particle at the interface and ratios of the viscosities of fluids.

The obtained results are summarized in graphs and tables, which can be used for calculation of the mobility of particles at interfaces and in independent experiments for determination of contact angles of micron-size objects attached to interfaces.

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Homogenization of the Heat Equation with a Vanishing Volumetric Heat Capacity

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We study the homogenization of the heat conduction equation with homogeneous Dirichlet boundary condition. The thermal conductivity is a periodically oscillating function of both spatial and temporal variables, reflecting the properties of the microscopic geometry. The volumetric heat capacity is a function, depending on a parameter ε, passing to zero as ε does. To prove a homogenization result we apply generalizations of multiscale and very weak multiscale convergence ([1]), made to include temporal oscillations. We use an approach which utilize a condition different from the standard assumption of boundedness of the time derivative. It turns out that the dependence of ε in the volumetric heat capacity and its matching with the microscopic scales give rise to certain special effects, as will be shown in the homogenization result.

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Instability and Heterogeneous Steady State in a Degenerate Chemotaxis Model

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The term chemotaxis is commonly used to describe the movement of a species or organism which has a tendency to aggregate by moving towards higher concentrations of chemical substances that they themselves produce. The first mathematical model describing chemotaxis at population level was proposed in 1970's by Keller- Segel [1] whose model provided a cornerstone for all subsequent mathematical modeling of chemotaxis [2, 3]. It consists of two parabolic equations: the first equation describes the cell dynamics and comprises a diffusive flux modeling random motion of cells, and an advective flux modeling directed cell movement with velocity proportional to the concentration gradient of the chemical, while the second equation is a reaction-diffusion equation describing the chemical kinetics with linear production and degradation with constant rates.

Our motivation is the study of the asymptotic behavior of solutions of a modified degenerate nonlinear Keller-Segel model. We show that the nonlinear evolution of a small perturbation around an homogeneous steady state is controlled by a finite number of fastest linear growing modes of this perturbation. Otherwise, we prove that the behavior of the nonlinear solution is similar to a heterogeneous stationary solutions, which gives a mathematical description of pattern formation. Then, we present a stable and convergent numerical scheme using a finite volume method [4] for the discretization of the Keller-Segel model. Finally, we investigate different numerical results in two dimensions to illustrate the effectiveness of our theoretical results presented in this paper and explore the pattern formation.

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An Improved Reservoir Model Calibration Using Sparsity and Stochastic Optimization

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Calibrating subsurface reservoir models with historical well observations leads to a severely ill-posed inverse problem known as *history matching*. In recent years, two fundamentally different methods for history matching have been proposed, namely gradient based methods on the one hand and stochastic ensemble based methods on the other. The recently proposed Ensemble Smoother Multiple Data Assimilation (ESMDA) [2] is such a stochastic technique. However, when applying it to large scale ill-posed inverse problems, computational complexity is still high and available prior information for example indicating a channel structure inside the reservoir is not automatically taken into account by its standard implementation.

In this work we propose a modification of the ESMDA which uses sparse dictionaries for reducing computational complexity and at the same time incorporating structural prior information. We use multiple point statistics (MPS) [4], with a suitable training image, to generate a set of equi-probable realizations of static properties of the reservoir satisfying the available structural prior information. This set of realizations is plugged into a K-SVD algorithm [1] combined with an orthogonal matching pursuit (OMP) technique [3] for generating an overcomplete dictionary representing typical reservoir parameters. Before starting the ESMDA, a sparse representation of a set of initial ensemble members is obtained by using this dictionary, which is then used throughout the ESMDA. The final estimates are then mapped back to the physical domain in order to analyse the results. We present numerical experiments on a modification of a standard SPE10 model in 3D that demonstrate that this novel algorithm outperforms standard ESMDA in preserving the assumed prior structural information on the reservoir and, moreover, performs faster due to the reduced number of unknowns in the sparse representation.

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Uncertainty Quantification of a Poroelasticity Model Using a Network-Inspired Porosity-Permeability Relation

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Fast, High Volume Infiltration (FHVI) is a new method to quickly infiltrate large amounts of fresh water into the shallow subsurface. This infiltration method would have a great value for the effective storage of rainwater in the underground, during periods of extreme precipitation. To describe FHVI, a model for aquifers is considered in which water is injected. Water injection induces changes in the pore pressure and deformations in the soil. Furthermore, the interaction between the mechanical deformations and the flow of water gives rise to a change in porosity and permeability, which results in nonlinearity of the mathematical problem. Assuming that the deformations are very small, the model provided by Biot's theory of linear poroelasticity with single-phase flow is used to determine the local displacement of the skeleton of a porous medium, as well as the fluid flow through the pores. The resulting saddle point problem needs a considerate numerical methodology in terms of possible spurious oscillations. Therefore, a Galerkin finite element method based on Taylor-Hood elements has been developed. In this continuum scale PDE model, the Kozeny-Carman equation is commonly used to determine the permeability of the porous medium from the porosity, which depends on the deformations. The Kozeny-Carman relation assumes that there will be flow through the porous medium at a certain location as long as the porosity is larger than zero at this location in the aquifer. In contrast, from discrete network models it is known that percolation thresholds larger than zero exist, indicating that the fluid will stop flowing if the average porosity becomes smaller than a certain value dictated by these thresholds. In this study, the difference between the Kozeny-Carman equation and the equation derived by Luis Lopez-Peña, based on the percolation theory, is investigated. Furthermore, we present results from Monte Carlo simulations that are performed to quantify the impact of variation in the soil characteristics, such as initial porosity and porous network topology, on the infiltration rate. We remark that our insights can be generally applied to flow in porous media with applications such as CO_2 sequestration and oil recovery.

Analysis of Multi-Species Biofilm Model

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In this talk we present our recent result on a well-posedness of a degenerate parabolic cross-diffusion model describing multi-species biofilm community. The model is proposed by Rahman, Sudarsan and Eberl in [1]. We discuss the global-in-time existence of weak solutions in a bounded domain with mixed Dirichlet-Neumann boundary conditions. The existence proof is based on an approximation argument, the entropy inequality and compactness lemmas. Moreover, based on the entropy inequality, the large-time asymptotics of the solution to the constant steady-state is shown. Furthermore, the uniqueness of solution is proved by combining the H^{-1}-method and the E-monotonicity technique of Gajewski. Finaly, we present some numerical simulations obtained using DUNE Numerics, the Distributed and Unified Numerics Environment which is a modular toolbox for solving partial differential equations with grid-based methods, [2].

Acknowledgments P. Milišić acknowledges the support of the scientific fund (grant HRZZ-IP-2013-11-3955).

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An Existence Theorem for Compositional Two-Phase Flow Model

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In this talk we present a system of equations governing liquid and gas flow in porous medium. The liquid phase is composed of liquid component and dissolved gas component, assuming low solubility of the gas component, while the gas phase is homogeneous. The model includes flow and transport of the components, diffusion in the liquid phase and the exchange of the mass between the phases given by the phase equilibrium relations. We formulate a weak solution of the initial-boundary value problem and prove existence theorem by approximating given parabolic system by a sequence of elliptic regularized systems, and by passing to the limit in the regularization parameters. The hypothesis of the gas component low solubility is given precise mathematical meaning.

Acknowledgments M. Jurak and A. Žgaljić Keko acknowledge the support of the scientific fund (grant HRZZ-IP-2013-11-3955).

Patents and Mathematics

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A short talk about patents and how to patent mathematical inventions. There will be a short introduction on what patents are, how to get them und what you can do with them once you have them. Although patents are a matter of national law, there are supranational mechanisms in place to make it easier to obtain patents for different countries. The focus will be on the European Patent Office (EPO) and its legal framework, the European Patent Convention (EPC) through which patents can be obtained for countries in Europe. We will look into more detail how mathematics can be turned into a patent and particular challenges Applicants need to be aware of. There will be some examples on inventions based on mathematics (mathematical inventions). Although some law will be required, we will keep this brief with emphasis on the practical/commercial sides of patents.

Numerical Fourier Transform Based on Hyperfunction Theory

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In this study, we propose a numerical method of the Fourier transform on hyperfunction theory, which is a theory of generalized functions [1] such as Dirac's delta functions. In hyperfunction theory, a hyperfunction $f(x)$ on an interval I is given by the difference of the boundary values of a complex analytic function $F(z)$, $f(x) = F(x + \mathrm{i}0) - F(x - \mathrm{i}0)$. In this theory, the Fourier transform of a function or a hyperfunction $f(x)$ is given by

$$\mathscr{F}[f](\xi) = \int_{-\infty}^{0} f(x)\mathrm{e}^{-2\pi\mathrm{i}(\xi+\mathrm{i}0)x}\mathrm{d}x + \int_{0}^{\infty} f(x)\mathrm{e}^{-2\pi\mathrm{i}(\xi-\mathrm{i}0)x}\mathrm{d}x = F_+(\xi + \mathrm{i}0) - F_-(\xi - \mathrm{i}0), \qquad (15)$$

where

$$F_\pm(\zeta) = \pm\int_{0}^{\infty} f(\mp x)\mathrm{e}^{\pm 2\pi\mathrm{i}\zeta x}\mathrm{d}x \quad (\pm\mathrm{Im}\,\zeta > 0\,).$$

In the presented method, we compute Fourier transforms as follows. First, we get $F_\pm(\zeta)$ in Taylor series $F_\pm(\zeta) = \sum_{n=0}^{\infty} \frac{1}{n!}F_\pm^{(n)}(\zeta_0^{(\pm)})(\zeta-\zeta_0^{\pm})^n$, where $\zeta_0^{(\pm)}$ are some fixed points such that $\pm\mathrm{Im}\,\zeta_0^{\pm} > 0$ and the coefficients $\frac{1}{n!}F_\pm^{(n)}(\zeta_0^{(\pm)})$ are obtained by conventional numerical quadrature rules such as the DE formula [3].

Table 1: The errors of the presented method and Sugihara's method [2] with the numbers of sampling points N

	N	error
presented method	2586	1.9×10^{-27}
Sugihara [2]	4018	2.0×10^{-18}

Second, we extend analytically $F_\pm(\zeta)$ onto the real axis by transforming them into continued fractions. Then, we obtain the Fourier transform $\mathscr{F}[f](\xi)$ by (15).
Table 1 shows an numerical example for

$$\mathscr{F}[|x|^\nu](\xi) = -2\sin\left(\frac{\pi\nu}{2}\right)\frac{\Gamma(\nu+1)}{(2\pi|\xi|)^{\nu+1}} \quad \text{with } \nu = 1.5 \text{ and } \xi = 1.$$

compared with Sugihara's method [2]. This shows the effectiveness of the presented method.
This work is supported by JSPS KAKENHI Grant Number JP16K05267.

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The Association of Bayesian Statistics and Monte Carlo Simulation in High Energy X-ray Radiography Reconstruction

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In a Core Punch experiment, the high energy x-rays is used to diagnose the compressed objects, including the edge determination and the density reconstruction. In the radiography analysis, the source of uncertainty are scatter which arises from the interaction of x-rays with matter and needs to be subtracted as these photons do not provide useful information, blur which results from the finite size of the x-ray source spot and the energy spread within the x-ray detector, and effect of the energy spectrum which comes from the source is not monoenergetic and hardening in the transmission. In order to improve the precision of reconstruction, a method which combined the Bayesian statistics and Monte Carlo simulation are used. In the present work, the experimental radiography will be given from the x-rays radiography experiment, and the simulated radiography is calculated by the Monte Carlo code which is used simulate the radiographic processes and considered the scatter parameters and source parameters and machine dose parameters. Then, the objective function is developed with the parameters are edge locations or density values, and the model parameters are varied to make sure the simulated radiography matches the experimental radiography. And the Bayesian statistics is employed to reject those solutions that are unphysical based on some prior knowledge such as mass conservation, non-negative density and density smoothness. Some experimental radiography with the samples like the multilayered-sphere and step are reconstructed by the above method, and more precious results are obtained. There are also some work needs to do in the future to optimize the methods such as introduce the Randomized Maximum Likelihood to save the calculation time and reduce the number of the parameters.

Acknowledgments The authors are grateful for the support of the National Nature Science Foundation of China (Grant No. 11505014).

A State-Expanded Model for the Bus Schedule Assignment Problem

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In our talk, we will present the bus schedule assignment problem for public transportation, which aims to assign the daily vehicle blocks to buses in the fleet of a transportation company over a longer planning horizon. This assignment has to satisfy the compatibility between bus-types and blocks, and must also consider vehicle-specific requirements: buses have to be sent parking at the end of each day, and their periodic maintenance activities should also be taken into account. In our earlier work [1], we introduced a model for this problem that examined parking as the only vehicle-specific constraint. This model was extended in [2] to consider maintenance activities as well, but solutions for larger problem sizes and longer planning horizons were computationally demanding. In this talk, we give a state-expanded multi-commodity flow network for the problem that considers all important vehicle-specific constraints (parking and maintenance), which is able to provide efficient solutions for larger problems as well. We compare the structure of this new model to the one presented in [2], and give an exhaustive comparison of their results on both real-life and randomly generated instances.

Acknowledgments Balázs Dávid acknowledges the support of the National Research, Development and Innovation Office - NKFIH Fund No. SNN-117879.
Miklós Krész acknowledges the European Commission for funding the InnoRenew CoE project (Grant Agreement #739574) under the Horizon2020 Widespread-Teaming program and the support of the EU-funded Hungarian grant EFOP-3.6.2-16-2017-00015.

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Change Point Detection for High-Dimensional Linear Regression and Its Applications for Covariance Matrices

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We pursue the goal of high-dimensional ($p > n$) covariance matrix estimation for data with abrupt structural changes. We try to detect these changes and estimate the covariance matrices in the resulting segments. Our approaches closely follow the proposal of Leonardi and Bühlmann [1] for change point detection in the case of high-dimensional linear regression. We consider the therein proposed estimator in more general setups and propose estimation procedures for covariance matrices based on this regression estimator, as well as another procedure, which is the analogy of the regression estimator, but directly for the case of covariance matrices. We present theoretical results, simulations for the comparison of these proposals, advantages and disadvantages, as well as an illustration of the developed methodology on a real-life example of stock returns.

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The Effect of the Type of the Elastic Foundation on the Dynamics of Track/Vehicle Systems

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We investigate the effect of various generalizations of the concept of elastic Winkler foundation to the motion of different kinds of loaded beams supported by discrete/continuous viscoelastic support systems. The beam is subjected to the action of static, fixed or moving loads. In the paper the closed-form analytical solutions obtained in earlier papers of the author and I. Zobory for the cases of Winkler and modified Winkler foundations are generalized to the case of more complicated foundation systems.

Posters

A Phase-Space Approach to the Propagation of Stochastic Fields

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In nature and technology, there are many complex sources, such as printed circuit boards (PCBs) that emit electromagnetic radiation that is stochastic. The modeling of such radiation is challenging and a long-standing research issue. We have developed theoretical methods to propagate noisy electromagnetic (EM) fields in free space. In our approach, we use the Wigner distribution function (WDF) to analyze radiation from complex sources in phase space. Our model helps characterize wave propagation both in the near field and far field. This is done by exploiting the relationship between the WDF and correlation function (CF). We also see that the Wigner function approach helps account for the evanescent components and their decay as we propagate the source CF [1]. Our model is validated through experimental results obtained using an Arduino microcontroller printed circuit board (PCB) as the source of stochastic fields. We have extended our model from 2D to 3D and proposed an improved near-field holography method [2].

The theoretical framework used for analyzing noisy EM emissions has some formal similarity to the formulation of the channel matrix of multiple input multiple output (MIMO) systems. We therefore propose that the WDF propagation technique may be adapted to be used as a means of providing information on the maximum achievable channel capacity in a given physical environment. A 2D rectangular waveguide is considered as an example for our analysis in this context.

Acknowledgments The authors acknowledge support from the European Commission through the Horizon 2020 FET project NEMF21,(grant 664828).

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Non-Renewable Fishery Resource Management Under Incomplete Information

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Population dynamics of fishery resources in natural environment is inherently stochastic. In addition, even if a stochastic model for their population dynamics has been identified, its model parameters are often uncertain. Stochastic optimal control under incomplete information [1] is a central mathematical tool for approaching the above-mentioned issue. Models that can potentially consider essential regime-switching phenomena of the body growth rate are especially of importance. The objective of this research is to formulate a stochastic optimal control problem for cost-effective management of an inland fishery resource under incomplete information where their body growth rate is uncertain. The population dynamics is described with a system of stochastic differential equations, and the dynamic programming principle leads to the Hamilton–Jacobi–Bellman (HJB) equation that governs the most cost-effective harvesting strategy of the fishery resource. Theoretical upper and lower-bounds of the value function, the objective function with the optimal harvesting policy, are derived. Demonstrative computational examples of the HJB equation based on a simple finite difference scheme [2] is presented focusing on *Plecoglossus altivelis* (*P. altivelis*, Ayu), a major inland fishery resource living in Japanese rivers. The regime-switching phenomenon of their body growth rate is assumed to be caused by temporal dynamics of the benthic algae, the main food source of the fish. The model parameters are identified for a river in Japan where the dynamics of *P. altivelis* and the benthic algae are the matters of high concern. Relationship between the regime-switching frequency and the optimal harvesting policy, which is characterized with a free boundary, is numerically explored.

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Comparison of Different Curve Fitting Settings During the Application of the Receptorial Responsiveness Method (RRM)

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A graded concentration-response (E/c) curve is an XY graph that relates the concentration of a substance to the response of a biological system. In the simplest case, the substance is an agonist that, once has bound to a specified macromolecule of the biological system called receptor, evokes a response. However, concentration of an agonist with short half-life in a given system is challenging to measure. One procedure to address this problem is the receptorial responsiveness method (RRM) [1]. RRM is based on a simplified mathematical modelling of the interaction between two agonists that consume the response capacity of the same biological system. Specifically, RRM enables the quantification of an acute increase in the concentration of an agonist with short half-life via constructing E/c curves with a stable agonist for the same system. This procedure results in a surrogate parameter of the surplus concentration in question, i.e. the equieffective concentration of the stable agonist. RRM can provide information about the change of agonist concentrations near the receptors, a compartment otherwise difficult to access [1]. In addition, RRM is suitable for the correction of experimental data obtained with the use of degradable agonists, and thus for computer simulation studies dealing with such issues [2]. In the present investigation, RRM was tested by evaluating experimental data, by means of using different settings for RRM according to three aspects: individual vs global fit, ordinary vs robust fit, and weighting (three types). This process yielded twelve outcomes, which were then compared to the expected result. Although the global fit offered the most convenient way to perform RRM, the best estimates were provided by the individual fit without any weighting, irrespectively of the fact whether ordinary or robust fit was chosen.

Acknowledgments This research was supported by the European Union and the State of Hungary (EFOP-3.6.2-16-2017-00015).

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Hypercomplex Fourier Transforms in the Analysis of Multidimensional Linear Time-Invariant Systems

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The classical signal theory deals with $\mathbb{R}$- or $\mathbb{C}$-valued functions and their $\mathbb{C}$-valued spectra. However, in some practical applications, signals tend to be represented by hypercomplex algebras [3]. Hypercomplex Fourier transforms deserve special attention in this considerations. Quaternion Fourier transform (QFT) allows us to analyse two dimensions of the sampling grid independently, while the complex transform mixes those two dimensions. It enables us to use the Fourier transform in the analysis of some 2-D linear time-invariant (LTI) systems described by some linear partial differential equations (PDEs) [2].

Recently, the notion of the octonion Fourier transform (OFT) of $\mathbb{R}$-valued functions of three variables has been introduced:

$$U_{\mathrm{OFT}}(f_1, f_2, f_3) = \int_{\mathbb{R}} \int_{\mathbb{R}} \int_{\mathbb{R}} u(x_1, x_2, x_3) e^{-2\pi \mathbf{e}_1 f_1 x_1} e^{-2\pi \mathbf{e}_2 f_2 x_2} e^{-2\pi \mathbf{e}_4 f_3 x_3} \, \mathrm{d}x_1 \mathrm{d}x_2 \mathrm{d}x_3, \tag{16}$$

where $\mathbf{e}_1$, $\mathbf{e}_2$ and $\mathbf{e}_4$ are three of the seven octonion imaginary units (each satisfying the property $\mathbf{e}_i^2 = -1$, $i = 1, \ldots, 7$ and other octonion multiplication rules). In previous investigations [1] it has been shown that (16) is well defined (i.e. the inverse transform theorem is valid). Some properties of the OFT, analogous to the properties of the complex and quaternion Fourier transform (e.g. Hermitian symmetry, shift theorem and Plancherel-Parseval theorems) were also derived.

In this presentation, the most recent results will be introduced, associating OFT with 3-D LTI systems of linear PDEs with constant coefficients. Properties of the OFT in context of signal-domain operations such as derivation and convolution of $\mathbb{R}$-valued functions will be stated. There are known results for QFT (see [2]), but they use the notion of other hypercomplex algebra, i.e. double-complex numbers. Results presented here require defining other higher-order hypercomplex structure, i.e. quadruple-complex numbers. This hypercomplex generalization of the Fourier transformation provides an excellent tool for the analysis of 3-D LTI systems.

Acknowledgments The research conducted by the author was supported by National Science Centre (Poland) grant No. 2016/23/N/ST7/00131.

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Coupled Simulation of Semiconductor Devices and Circuits in the THz Range

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Electromagnetic waves with a frequency in the range from 100 GHz to 10 THz are referred to as THz waves. They are difficult to generate, because their frequencies are on the one hand too high for efficient operation of state of the art solid-state devices and on the other hand too low for optical generators. Current THz sources filter out the third harmonic of an oscillator, leading to extremely low power efficiency. This led to the proposal of a new kind of solid-state devices based on plasma waves in quasi 2D electron gases, where the THz signal is generated directly within the device by the electron fluctuations. Since the dispersion relation of the plasma waves, their instabilities and the gain of the device depend on the geometrical structure, permittivity of the materials, dimensionality of the electron gas and its density, boundary conditions etc., it gives the device designer a lot of freedom and various device concepts have been proposed but yet not been realized.

The standard electron/hole transport models based on the Euler equation are generalized to describe the transport in THz regimes, e.g. by a convective term or moments of higher order (e.g. hydrodynamic model). This requires novel numerical algorithms ranging from generalizations of the Scharfetter-Gummel stabilization, numerical integration techniques for THz oscillations, e.g. trigonometric spline-wavelet methods, to iterative linear and nonlinear solvers for huge systems of equations.

The device behavior must be simulated within a circuit environment, since the signal power which can be decoupled depends on the termination of the device's ports and each individual configuration has to be simulated since the circuit behavior is nonlinear. Thus, a coupled device/circuit simulator is required to investigate nonlinear effects. To this end, the modular circuit simulator LinzFrame has been coupled with the semiconductor device simulator.

Acknowledgments This work has been partly supported by the DFG/FWF DACH project under grant I3130-N30. This project has been co-financed by the European Union using financial means of the European Regional Development Fund (EFRE). Further information to IWB/EFRE is available at www.efre.gv.at.

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An Unconstrained Minimization Technique Using Successive Implementations of Golden Search Algorithm

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In this paper, we propose a new technique in solving the minimum of a function defined on a ball centered at x^0 with radius $\overline{\rho}$ using successive implementations of Golden Search algorithm. We show numerically that our proposed method can effectively approximate the minimum of a function even if it is nonsmooth or discontinuous. We also introduce partitioning to estimate the global minimum of multimodal functions. Furthermore, we apply our method to estimate the parameters of a physiological system.

Acknowledgments The authors are grateful for the support by the Department of Science and Technology - Science Education Institute (DOST-SEI) Accelerated Science and Technology Human Resource Development Program - National Science Consortium (ASTHRDP-NSC) Student Research Support Fund Dissemination Grant.

A Three-Step Approach to Edge Detection of Texts

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We propose a three-step image segmentation approach to determine the edges of images containing old texts. In general, texts from old books and articles tend to be very noisy. Thus, we first use L^2-Regularization to obtain a smooth approximation I_s of a given image $\tilde{I}$. Then, the fuzzy edge map $\tilde{E}$ is obtained using the gradient of I_s. This gradient map will give an estimate of the edges of the texts. For the second step, the method of `K-means++` with two clusters is employed to separate the edges from rest of the image. Because a smooth approximation of the image is used, the edges obtained are "thick". And so in the last step of the proposed method, the binary image generated from the previous step is post-processed using a thinning algorithm. We implement our proposed algorithm to images, containing *baybayin* texts, from the Philippine National Museum.

Acknowledgments The authors are grateful for the financial support by the Department of Science and Technology-Science Education Institute (DOST-SEI) Accelerated Science and Technology Human Resource Development Program-National Science Consortium (ASTHRDP-NSC) Student Research Support Fund (SRSF) Dissemination Grant.

Multiplicity of Nontrivial Solutions for Perturbed Fourth Order Kirchhoff Type Elliptic Equations

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The elliptic equation $-M(\int_\Omega |\nabla u|^2\, dx)\triangle u = f(x,u) in \Omega$ is related to stationary problem

$$\rho\frac{\partial^2 u}{\partial t^2} - (\frac{\rho_0}{h} + \frac{E}{2L}(\int_0^L \left|\frac{\partial u}{\partial x}\right|^2 dx))\frac{\partial^2 u}{\partial x^2} = 0.$$

It is an extension for the classical D'Alembert's wave equation for free vibrations of elastic strings, see [1]. In this poster, we consider the following perturbed fourth-order Kirchhoff type elliptic equation: let $M : [0,\infty) \to R$ be a continuous function, $f : \Omega \times R \to R$ be a Caratheodory function, and

$$\begin{cases} \triangle^2 u - M(\int_\Omega |\nabla u|^2\, dx)\triangle u + \rho u = \lambda f(x,u) \quad in\ \Omega; \\ u = \triangle u = 0 \quad on\ \partial\Omega, \end{cases}$$

where λ, $\mu > 0$, $\Omega \subset R^N$ is a bounded domain with smooth boundary $\partial\Omega$. In [2], we know that the fourth-order elliptic equation of nonlinearity furnishes a model to study travelling waves in suspension bridges. By using the variational methods and critical point theory, we investigate the multiplicity of nontrivial solutions for this equation.

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Finite Element Simulation of Transducer with Plano-Concave Face from Nanostructured Porous Piezoceramics

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In the recent time an increased interest has been observed to the investigations of piezocomposite materials that exhibit very effective properties for many applications.

The first part of our research concerns direct finite element modeling of piezoelectric two-phase composites. The proposed technique is based on the models of nanoscale materials with surface effects, the effective moduli method, modeling of representative volumes and the use of finite element technology. As particular case we investigate the nanoporous piezoceramic materials. For these materials we use the special models of representative volume, take into account the surface effects on the boundaries of nanosized pores. Here, we apply the Gurtin-Murdoch model of surface effects with special conditions for stresses at the borders between piezoelectric material and pores. In second part to increase the efficiency of electro-mechanical transformation it is proposed to use the circular transducer from nanostructured porous piezoceramics in which one of its end surfaces has a plano-concave shape. We suppose that this transducer will have greater flexibility for bending deformation and, as a consequence, will have large effective piezomoduli.

In the computational experiments the plane-concave transducers with electrode face plates made from nanostructured porous piezoceramics PCR-1 have been examined. The effective thickness piezomodule d_{33} was obtained in quasi-static tests with a force F applied at the center of the top plane surface. The transducer was placed on the foundation, leaning on the flat part of its bottom end surface of the plano-concave form. Under the action of the force F the transducer was deformed, and due to the piezoelectric effect the electric charges Q have appeared on the electrodes. The effective thickness piezomodule was defined as the ratio of the induced charge to the applied force: $d_{33}^{\text{eff}} = Q/F$.

For the proposed plano-concave disk circular transducer we were carried out the finite element modeling using ANSYS. We have built solid and finite element models of the considered transducer in the axisymmetric statement. Developed programs allowed to calculate the effective thickness piezomoduli for different geometrical and physico-mechanical input data and for different size of porosity under static and harmonic analyses.

Since the experimental and computation results have shown a good agreement for the test samples, that it allows to predict the effective properties of a plano-concave transducer for various input data by using the appropriate computer calculations. Naturally, the effective piezoelectric moduli increase with decreasing of disk height and with increasing of concavity radius. So, for the certain input data we have obtained an increase of the effective thickness piezomodule compared with the piezomodule of dense material a hundreds time, that it opens up the various possibilities of using the new circular piezoelectric transducer for different applications.

Acknowledgments The reported study was funded by RFBR according to the research project 16-01-00785.

Perfect Landmark Sets in the Alt Route Planning Algorithm

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We study the problem of finding a the shortest path. One of the most used algorithm is A^* algorithm. However it requires a function called a potential which assigns to each vertex v a lower bound on the distance from v to the target. Usually the potential is based on some additional properties of a graph, e.g its geometrical representation. A universal approach to constructing a useful potential function is to choose an arbitrary subset L of the vertices, called a landmark set, and precompute the distances from each landmark to every vertex of the graph. Using the triangle inequality we obtain $\mathrm{dist}(v,t) \geq \mathrm{dist}(v,l) - \mathrm{dist}(t,l)$ for every vertex v and landmark l, where t is the target. It follows that $\pi(v) = \max\{|\mathrm{dist}(s,l) - \mathrm{dist}(t,l)| : l \in L\}$, is a viable potential function. This approach is called ALT (A for A^*, L for landmarks and T for triangle inequality) [2]. Note that adding more vertices to L may result in a more useful potential π, but π is computed in time $O(|L|)$ and uses auxiliary data that takes $O(|L|\,|V(G)|)$ memory, so we want to keep the number of added vertices as low as possible.

If we fix the number of landmarks then the problem of choosing optimal landmark set is NP-hard [1]. Our approach is complementary: to find a perfect landmark set L of minimum cardinality. We say that L is perfect if for any two vertices s,t there exists a vertex $l \in L$ such that $\mathrm{dist}(s,t) = |\mathrm{dist}(s,l) - \mathrm{dist}(t,l)|$. It means that the distance between any vertices s,t is given by the formula $\mathrm{dist}(s,t) = \max\{|\mathrm{dist}(s,l) - \mathrm{dist}(t,l)| : l \in L\}$ and can be computed in $O(|L|)$ time using $O(|L|\,|V(G)|)$ precomputed data. If L is small then we obtain a very fast implementation of the ALT algorithm finding a shortest path.

Although the problem of finding the cardinality of a smallest perfect landmark set is NP-hard, it can be effectively approximated. We give a 2-approximation algorithm. Notice that a perfect landmark set even twice bigger than the smallest still gives us an $O(|L|)$-time algorithm for the shortest path problem.

We have also observed that sometimes the size of a minimum perfect landmark set can be significantly reduced by adding some extra vertices to the graph, which gives a further increase in performance of the computation of shortest paths. There are examples of graphs with arbitrary large minimum perfect landmark set that are isometric subgraphs of a graph with a small (e.g 2-element) perfect landmark set. This means that the ALT algorithm can be efficiently used for much larger classes of graphs.

Acknowledgments Research funded by the grant H2020 688380.

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Lane Modelling Algorithm for Video-Based Driver Assistance System

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In traffic situations it is crucial to have as complete description about the traffic lanes as possible in both driver assistant (DA) and automated driving (AD) systems. Lane estimation is based on environment model built from sensor data and used for course estimation for ego vehicle and behavior prediction of traffic participants in neighbouring lanes.

In video-only DA systems, the input for lane modelling algorithm consist of e.g. free space information, segmented video lanes with several attributes, like color, confidence. As a first processing step, the road geometry can be investigated via exploring connectivity relation between different lane segments to obtain estimation for lane borders. This approach allows constructing several possible courses, which is essential in complex situations like construction zones, where classical parallel lane models are not applicable.

In this work, the connectivity relation is represented by a weighted graph, where the nodes are the lane segments and link weights are calculated with a similarity function, which incorporates common Gestalt principles for e.g. continuity, alignment. As a naive approach, the elements of the weighted neighborhood matrix can be transformed to binary via thresholding to obtain a simple graph and connected components of the graph form clusters, which provides basis for curve fitting algorithm approximating lane borders. A more sophisticated approach applies spectral clustering on the weighted graph, which strongly relates to spectral drawing of graphs. A combination of these concepts leads to a new and efficient method, which is easily interpretable and controllable.

In the cooperation with Robert Bosch Kft., we have access to measurement campaigns to evaluate implemented algorithms.

Acknowledgments The research is supported by the EU funded Hungarian grant project Nr. EFOP-3.6.2-16-2017-00015.

Mathematical Analysis and Numerical Methods
for Internal Incompressible Flows with Inertial-Dissipative Inflow/Outflow Conditions

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Numerical modeling of incompressible unsteady flows is a big challenge both in theoretical terms (i.e. study of existence and uniqueness of solutions) and more practical ones (i.e. implementation of algorithms). Numerical solution to given problem usually requires bounded domain (despite the fact that problem might be defined on wider than implemented or even unlimited domain). In the literature different ways to deal with this problem are described (see [1], [2]). In this presentation we will focus on the model proposed by prof. Jacek Szumbarski.
We consider unsteady Stokes problem in domain Ω described by the system:

$$\begin{cases} \partial_t \boldsymbol{u} - \nu \Delta \boldsymbol{u} + \nabla p = g, \\ \nabla \cdot \boldsymbol{u} = 0, \end{cases}$$

where the boundary $\partial\Omega$ consist of rigid, impermeable wall Γ_0 and inlet/outlet sections Γ_k, $k = 1, \ldots, K$. The boundary conditions are defined as follows:

$$\boldsymbol{u} = 0 \quad \text{on } \Gamma_0, \tag{17}$$

$$p\boldsymbol{n} - \nu \nabla \boldsymbol{u} \cdot \boldsymbol{n} - \boldsymbol{u} \left(\lambda_k + \gamma_k \frac{\mathrm{d}}{\mathrm{d}t} \right) \Phi_k(\boldsymbol{u}) = S_k \boldsymbol{n} \quad \text{on } \Gamma_k,\ k = 1, \ldots, K, \tag{18}$$

$$p\boldsymbol{n} - \nu \nabla \boldsymbol{u} \cdot \boldsymbol{n} - \boldsymbol{u} \left(\hat{\lambda}_k + \hat{\gamma}_k \partial_t \right) (\boldsymbol{u} \cdot \boldsymbol{n}) = S_k \boldsymbol{n} \quad \text{on } \Gamma_k,\ k = 1, \ldots, K, \tag{19}$$

where Φ_k is flowrate operator, e.g. $\Phi_k(\boldsymbol{u}) = \displaystyle\int_{\Gamma_k} \boldsymbol{u} \cdot \boldsymbol{n} \, \mathrm{d}\mathcal{S}$ and coefficients $\{\lambda_k, \gamma_k\}$ in (18) or $\{\hat{\lambda}_k, \hat{\gamma}_k\}$ in (19) are defined for all $k = 1, \ldots, K$. Further, we assume that also given are the functions $\{S_1(t), \ldots, S_{K_p}(t)\}$, while the functions $\{S_{K_p+1}, \ldots, S_K(t)\}$ should be found. Initial condition for velocity field is $\boldsymbol{u}(t = 0) = u_0$.
This is a preliminary model which can be applied to simulate flows in cardiovascular and respiratory systems. In addition to physical considerations over correctness of given model, we will focus on describing the method of finding the solution and presenting results related to existence and uniqness of solution.

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