Abstracts

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Contents

ECMI 2014

Mini-Symposium on Spacetime Models of Gravity in Geolocation and Acoustics.

José María Gambi [1] [2]*, Michael M. Tung* [3] [4] *and Manuel Carretero* [5]*.*

Description and relevance to ECMI

The geometrization of gravity forms one of the cornerstones of modern science having an impact on the industrial progress connected to many activities of daily life. In the past decade, substantial research has been invested into post-Newtonian corrections for high-precision navigation, geolocation, and tracking devices, as well as into the design of analogue models of gravity by making use of advanced optical and acoustic metamaterials. Present industrial needs demand innovative development of computationally efficient spacetime models in this interdisciplinary field. Such mathematical models become important for applications requiring very accurate timing as achieved in todays engineering systems which rely on modern atomic clocks. Moreover, acoustic metamaterials–artificially produced with properties not found in nature–challenge the engineer to fabricate acoustic devices with highly unusual features. Therefore, we do believe that this proposed mini-symposium could significantly contribute to the ECMI 2014 Conference agenda being in line with its major goals.

Confirmed speakers

- José María Gambi (Univ. Carlos III de Madrid)
- Michael M. Tung (Univ. Politécnica de Valencia)
- María Luisa García del Pino (Univ. Carlos III de Madrid)
- Mariá del Carmen Rodríguez-Teijeiro (Univ. Carlos III de Madrid)
- Javier Clares (Univ. Politécnica de Madrid)
- Rafael Olmedo (GekoNAVSAT S.L.)

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Other proposed speakers

- Emilio Defez (Univ. Politécnica de Valencia)

Industrial participation

GekoNAVSAT is a technology-oriented company focussing on the development of industrial solutions based on global navigation satellite systems. Due to its social and economic relevance, the company is located on the premises of the Parque Científico of the Univ. Carlos III de Madrid.

Mini-Symposium on Imaging and inverse problems

A. Carpio (UCM), M.L. Rapun (UPM).

Imaging problems appear in many real life applications, for example, med- ical imaging, material testing, geophysical or astrophysical studies. Depending on the context, these problems may adopt different mathematical forms. Often, information about objects is to be found from knowledge of the influence that those obstacles have on propagating waves. A different situation arises when an existing image or signal has to be restored to remove noise. In this minisimpo- sium, we present a summary of recent results in both frameworks.

P. Gonzalez (UC3M) will discuss optical imaging of tissues. A. Marquina (UV) analyzes the reconstruction of noisy and blurry signals by means of L^1 regularizations. S. Serna (AUB) pursues this topic resorting to total varia- tion image restoration. M.L. Rapun (UPM) considers photothermal imaging. Finally, V. Selgas (UNIOVI) presents some results on scattering by dielectric objects.

Their titles and abstracts are listed below.

The Inverse source problem in mesoscopic scattering regimes using angle-resolved measurements

P. González-Rodríguez
Universidad Carlos III

We study optical imaging of tissues in the mesoscopic scattering regime in which light multiply scatters in tissues, but is not fully diffusive. Our purpose is to show that, in this regime, using angle-resolved data improves the results considerably. To prove this we compare the solution of two similar inverse source problems that are solved using the same ℓ^1-optimization method. In the rst problem we nd a solution of a linear system $Ax = b$ in wich the initial entries $A_{i,j}$ of the matrix are the scalar ux response at a boundary grid point ρ_i due to an isotropic point source r_i governed by the radiative transport equation. Once the matrix is calculated, we normalize the columns. The right hand side b is the angle averaged data. The second problem $Bx = c$ is similar, but in this case the entries $B_{i,j}$ of the matrix are the directional response at a boundary grid point ρ_i due to an isotropic point source r_i also governed by the radiative transport equation. As with A, we normalize the columns of B. The right hand side c represents the angle-

resolved measurements. We show that recovering the location and strength of several point-like sources is not possible when using angle-averaged measurements, while just using two angled-resolved measurements the results are improved radically. In both problems, the matrices A and B are calculated efficiently computing the RTE Greens functions as an expansion of plane wave solutions.

Variational Models and Numerical Algorithms for one-dimensional Signal Reconstruction of Noisy and Blurry Signals: Application to the signal recovery for future detection of Gravitational Waves

Antonio Marquina
Universidad de Valencia

In this research work we examine the one dimensional variational models for reconstruction of signals using L^1-regularizations. We present an analysis of the variational models based on L^1-regularization and we implement numerical algorithms that allow to recover noisy and blurry signals, using direct methods and regularization procedures. We shall present an application for the recovery of one-dimensional signals to be observed in the near future in different gravitational wave detectors.

The regularized split Bregman method based on rational approximations of the absolute value function for total variation image restoration

Susana Serna
Universidad Autónoma de Barcelona

We explore the regularization of the shrinkage function based on an approximation of the absolute value function to design a class of split Bregman methods for total variation image restoration. We introduce a hierarchy of regularizations depending on a positive parameter that determines the accuracy in the approximation of the absolute value function by rational functions. We present a set of numerical tests involving the restoration of signals and synthetic images contaminated with noise and blur.

Domain and parameter reconstruction in photothermal imaging

Ana Carpio (Universidad Complutense)
MaríaLuisa Rapún (Universidad Politécnica de Madrid)

Photothermal imaging aims to reconstruct the inner structure of materials by heating their surface using a laser beam and recording the surface temperature. The goal is to detect structural defects or inclusions (determine their location, size, shape, orientation) and their nature (physical parameters).

In this work we propose an iterative descent method that combines topological derivative computations to reconstruct the geometry of the defects with gradient iterations to approximate the material parameters.

Some numerical experiments showing the ability of the method to obtain reasonable reconstructions in a few iterations will be shown. Furthermore, we numerically corroborate that a small number of sampling points and source points allow for reliable reconstructions if we record the temperature during a time interval.[6]

Transmission eigenvalues for a dielectric object resting on a perfect conductor

Peter Monk (University of Delaware)
Virginia Selgas (Universidad de Oviedo)

We introduce a new transmission eigenvalue problem with mixed boundary conditions that arises when a dielectric scatterer is mounted on a metal structure.

Indeed, we describe the forward problem and show that it has a unique solution using a reflection principle. We also formulate the inverse problem of identifying the shape of the dielectric from near field measurements. To solve numerically this inverse problem, we propose the standard near field Linear Sampling Method (LSM); notice that the equations involved in the

[6] **References**:
(1)A. Carpio and M.L. Rapún (2008), Domain reconstruction using photothermal techniques. J. Comput. Phys., 227. 8083-8106.
(2)A. Carpio and M.L. Rapún (2013), Parameter identification in photothermal imaging, JMath Imaging Vis, to appear. DOI 10.1007s10851-013-0459-y.

LSM and in the approximation of transmission eigenvalues from measurements are one and the same.

Moreover, we reformulate the mixed transmission eigenvalue problem as a fourth order partial differential equation. Then we show that there exist infinitely many transmission eigenvalues and derive monotonicity as well as a lower bound estimate for the first eigenvalue. Our analysis mainly uses tech- niques from (4, 1, 2), and requires us to prove suitable density and compactness properties.

We also provide numerical examples for the LSM; and finally demonstrate that, for the cases we have considered, mixed transmission eigenvalues can be approximated from near field data; see (3) for a study of the corresponding far field problem for standard transmission eigenvalues. [7]

[7] **References**:

(1)F. Cakoni and H. Haddar, A variational approach for the solution of the electromagnetic interior transmission problem for anisotropic media, Inverse Problems and Imaging 2007(1), 443-456.

(2)F. Cakoni and H. Haddar, On the existence of transmission eigenvalues in an inhomogeneous media, Applicable Analysis 2009(88), 475-493.

(3)A. Cossonnière, PhD thesis, Valeurs propres de transmission et leur utilisation dans lidentification dinclusions a partir de mesures électromagnétiques, Université de Toulouse 2011.

(4) H. Haddar, The interior transmission problem for anisotropic Maxwells equations and its applications to the inverse problem, Math. Meth. in the Appl. Sci. 2004(27), 2111-2129.

(5) P. Monk and V. Selgas, Transmission Eigenvalues for Dielectric Objects on a Perfect Conductor, Inverse Problems 2013(29), 104007.

Mini-Symposium on Computational Finance

Matthias Ehrhardt (Bergische Universität Wuppertal)
Jörg Kienitz (Postbank AG, Bonn)
Jan ter Maten (Bergische Universität Wuppertal, TU Eindhoven)

In recent years the computational complexity of mathematical models employed in financial mathematics has witnessed a tremendous growth. **Advanced numerical techniques** are imperative for the most present-day applications in financial industry. The aim is to **deeper understand complex (mostly nonlinear) financial models and to develop effective and robust numerical schemes for solving linear and nonlinear problems** arising from the mathematical theory of pricing financial derivatives and related financial products. The motivation for this minisymposium is to exchange and discuss current insights and ideas, and to lay groundwork for future collaborations. Finally, it should serve as a kickoff for the special interest group (SIG) Computational Finance.

Speakers (confirmed)

- Alfio Borzi (Würzburg): *A Fokker-Planck-Kolmogorov control framework for Ito stochastic processes and piecewise-deterministic processes*
- Maria Grossinho (Lisbon): *A class of nonlinear boundary value problems for a Black-Scholes type equation*
- Christoph Reisinger (Oxford): *Numerical solution of stochastic PDEs arising in financial engineering*
- José Germán López Salas (A Coruña): *Efficient calibration and pricing in recent SABR-LIBOR Market Models using GPUs*
- Christof Heuer (Sussex): *High-order compact finite difference schemes for parabolic differential equations with mixed derivative terms in n space dimensions and application to basket options*
- Marta Pou Bueno (Delft): *Fourier-Cosine method to solve Backward Stochastic Differential Equations in recent finance aspects*
- Zuzana Bučková (Wuppertal): *Fichera theory and its application*
- Pedro Polvora (Bratislava): *Extensions of the Barles and Soner model for derivatives pricing with transaction costs*

- Vera Egorova (Valencia): *A Positive, stable and consistent front-fixing numerical scheme for American Options*
- Walter Mudzimbabwe (Ruse): *An efficient Monte Carlo algorithm for pricing arithmetic Asian options under a jump diffusion process*
- Nicola Cantarutti (Lisbon): *Option pricing in exponential Levy models with transaction costs*
- Ivan Yamshchikov (ZittauGörlitz): *Portfolio optimization in the case of an asset with a given liquidation time distribution*
- Lara Trussardi (Vienna): *Analysis of a herding model in social economics*
- Fernando Goncalves (Lisbon): *Discretisation of degenerate PDEs with unbounded coefficients in finance*
- Mohamed El-Fakharany (Valencia): *Numerical solution of Partial-Integro Differential option pricing models with cross derivative term*
- Yaser Kord (Lisbon): *Approximation of one-dimensional degenerate PDEs in unbounded domains related to finance.*

Mini-Symposium on Mathematical Modelling in Energy Markets

Michael Coulon (University of Sussex)
Matthias Ehrhardt (Bergische Universität Wuppertal)

The rapid changes in energy trading within the last two decades have attracted many researchers in academia and industry. Their aim is to adequately model energy prices and typically also to design methods and guidelines for risk management challenges such as power plant portfolio optimization.

The well-known non-storability property of electricity (and challenges in natural gas storage) leads to major modelling differences compared to stock or bond markets. Coupled with highly inelastic demand and a variety of supply side constraints, this lack of storage can result in sudden price spikes and high, time-varying volatility. Furthermore, mean reversion rates and typical seasonal patterns exhibit a complex multi-scale nature with respect to the time variable: intra-day, weekly and annual.

The aim of this minisymposium is to discuss the latest research in industry and academia in energy modelling and energy risk management. It will cover different modelling approaches for energy prices with particular focus on applications in gas and electricity markets.

Speakers (confirmed)

- Michael Coulon (University of Sussex): *An Introduction to Mathematical Models in Energy Markets*
- Nina Lange (Copenhagen Business School): *Currency Risk in Energy Markets*
- Virginie Dordonnat (EDF): *Nonparametric modelling and short-term forecasting of French electricity demand and spot prices*
- Christian Jacobsson (Alpiq, Lausanne): *Optimizing day-ahead/intraday trading of uncertain renewables production and flexible hydro*
- Christian Hendricks (University of Wuppertal): *Clean Spread Options in the German Electricity Market*
- Alexander Boogert (EnergyQuants, Amsterdam): *A practical perspective on gas storage*

- Magnus Wobben (d-fine AG, Frankfurt): *Valuation of Storage Contracts in Incomplete Gas Markets*
- Sven-Olaf Stoll (EnBW, Karlsruhe): *A model for coupled spot and forward prices for natural gas*

Mini-Symposium on Industrial Particle and Interface Dynamics

Dr. Tuoi Vo T.N. [8] [9]

This mini-symposium will focus on mathematical modelling of processes occurring at interfaces and in particulate systems which arise in industry (for example, food and drink, pharmaceutical, and other sectors). These challenging industrial problems are currently under investigation at the Mathematics Application Consortium for Science and Industry (MACSI) in Ireland. The talks will cover the development of innovative mathematical models to help industry optimise and improve processes, increase scientific understanding, and meet regulatory requirements. Models are developed for chemical extraction from powdered substrates, and particle motion and adhesion in circulating flows. Asymptotic, analytical and numerical techniques are used to investigate the mathematical models.

Motivation/Relevance to ECMI

Particles and interfaces are ubiquitous in industrial processes. The talks will cover applications to industrial processes in the food and drink, pharmaceutical, and other sectors. Although under investigation in Ireland, the problems are of interest in a wider European context also.

Speakers (confirmed)

- Tuoi Vo T.N., University of Limerick, Ireland
- William Lee, University of Limerick, Ireland
- Kevin Moroney, University of Limerick, Ireland
- Brendan Florio, University of Limerick, Ireland.

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Mini-Symposium on Methods for Advanced Multi-Objective Optimization for eDFY of complex Nano-scale Circuits

Salvatore Rinaudo, CAD and Design Services Director, STMicroelectronis S.r.l.
Giuliana Gangemi, CAD and Design Services Program Manager, STMicroelectronis S.r.l. [10]

Short Description

Cost control, production efficiency, cycle time and yield are critical quality benchmark for nano-electronics productions. An increasingly important downside of nano-CMOS technology scaling is the fact that the scaling of feature sizes cannot be accompanied by a suitable scaling of geometric tolerances. In addition, when getting into deep miniaturized dimensions, phenomena like edges or surfaces roughness, or the fluctuation of the number of doping atoms within the channels are becoming increasingly significant. As a result, the figures of merit of a circuit, such as performance and power, have become extremely sensitive to uncontrollable statistical process variations (PV).

To ensure stable manufacturability and secure high manufacturing yield, it is mandatory to manage complete design flows and to link traditional methods for design with Technology CAD models. In this context, **multi-objective optimization algorithms and statistical analysis** are essential on device and behavioural levels to secure high yielding by modelling the impact of inevitable process variations and doping fluctuations on IC performance. Statistical circuit modeling is a viable solution to nano-electronics production quality.

We propose a mini symposium on Methods for Advanced Multi-Objective Optimization for eDFY of complex Nano-scale Circuits developed, tested and implemented within the MANON project, this special session shall give an overview of the challenges and of the methodological solution to the above issues implemented by the MANON consortium.

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The scope of the research activity has been to create PV-aware and PV-robust circuit design techniques, tools and models in the frame of the analogue and mixed-signal circuit industrial design.

Academic and industrial state of the art optimization and methods to generate circuits behavioral models have been studied and analyzed on selected industrial test cases. The research activities started from the analysis of what is currently the state of art in the industrial design flow for the generation of eDFY models and from its limitations. The selected test-case, because of the high order non-linearities as well as for the huge number of process parameters needed to properly characterize the performance behavior in the parameter space, didnt allow the generation of accurate eDFY models with the EDA tool Wicked which is based on the Response Surface Methodology (RSM).

For this reason, three new different methodologies have been investigated in this project and the different pro and cons are reported below.

The methodologies taken into account are

1. A combination of *Support Vector Machine (SVM)* or *Neural Networks (NN)* surrogate models and a *Derivative-free mixed-integer black-box optimization* algorithm to be used for faster circuits yield estimation.

2. The usage of *Symbolic Model Order Reduction (SMOR)* techniques for reducing the complexity of the system of differential equations describing the behavior of an integrated circuit, thus reducing drastically the simulation time.

3. Enhance the RSM models accuracy using RBF (radial basis functions) with automatic width variation, per function and/or input parameter. In addition, research into *table-based models* enabling: run-time check of coverage, incremental model updates, *Global Process Variation (PV)* using interpolated sensitivity matrix, mismatch using interpolated covariance matrix and new performance distributions.

4. The usage of NN to reduce simulation time of transient analyses while execution of a Monte Carlo analysis.

Motivation/Relevance to ECMI

The MANON project is the success story of a long lasting joint venture amongst academies, industry and SME to develop the mathematical know how on multi-objective optimization, symbolic techniques and numerical

statistical simulation and to apply it to industry strength test cases with Electronic Design Automation (EDA) software modelling skills.
The project is funded by the Europen Union within the 7th Framework Program, with Grant Agreement FP7 MCA IAPP no. 251380.
The presentations we propose are in part directly related to the MANON research outcomes and their industrialization i.e. the implementation of the mathematical results in a prototype tool that make the science available to the technological industrial advances.
The presentations made by Prof Lucidi and Prof Graeb have a broader theoretical scope, still related to the scientific topics covered by the MAnON project, such as multi objective optimization, Analog Design Centering and Sizing as well as Reliability Optimization. Their purpose is to give more insight into specific mathematical problems which needs to be applied to circuit analysis, sizing and optimization and could be inspirations for future researches.

Speakers (confirmed)

- Giuliana Gangemi, Salvatore Rinaudo, STMicorelectronics: *The MANON project.*
- M.A. Khozoei, ITWM Fraunhofer Institute: *The usage of Neural Networks to reduce simulation time of transient analyses while execution of a Monte Carlo analysis.*
- Zia Abbas, Sapienza University: *Application of mathematical methods to the modeling of logic cell performance.*
- Vittorio La Torre, Gianni Di Pillo, Sapienza University: *Yield optimization in electronic circuits design.*
- M.A. Khozoei, P.Lang, ITWM Fraunhofer Institute: *The usage of Symbolic Model Order Reduction (SMOR) techniques for reducing the complexity of the system of differential equations describing the behavior of an integrated circuit, thus reducing drastically the simulation time.*
- Carlo Roma: *MunEDA Fast Monte Carlo for Circuit Design.*
- Carmelo Vicari, Angelo Ciccazzo STMicroelectronics: *A Wicked based framework for circuit modelling and statistical circuit optimization.*

- Helmut Graeb, Technische Universitaet Muenchen: *How can we include Pareto front computation, discrete parameter values and aging into analog circuit sizing?.*

- Stefano Lucidi, Sapienza University: *Derivative-free methods for multiobjective Lipschitz problems.*

Guest speakers

Helmut Graeb got his Dipl.-Ing., Dr.-Ing., and habilitation degrees from Technische Universitaet Muenchen in 1986, 1993 and 2008, respectively.
He was with Siemens Corporation, Munich, from 1986 to 1987, where he was involved in the design of DRAMs. Since 1987, he has been with the Institute of Electronic Design Automation, TUM, where he has been the head of a research group since 1993.
His research interests are in design automation for analog and mixed-signal circuits, with particular emphasis on Pareto optimization of analog circuits considering parameter tolerances, analog design for yield and reliability, hierarchical sizing of analog circuits, analog/mixed signal test design, discrete sizing of analog circuits, structural analysis of analog and digital circuits, and analog layout synthesis.
Dr. Graeb has, for instance, served as a Member of the Executive Committee of the ICCAD conference, as a Member or Chair of the Analog Program Subcommittees of the ICCAD, DAC, and D.A.T.E conferences, as Associate Editor of the IEEE TRANSACTIONS ON CIRCUITS AND SYSTEMS PART II: ANALOG AND DIGITAL SIGNAL PROCESSING and IEEE TRANSACTIONS ON COMPUTER-AIDED DESIGN OF INTEGRATED CIRCUITS AND SYSTEMS, and as a Member of the Technical Advisory Board of MunEDA GmbH Munich, which he co-founded. He is a Senior Member of IEEE (CAS) and member of VDE (ITG).
He was the recipient of the 2008 prize of the Information Technology Society (ITG) of the Association for Electrical, Electronic and Information Technologies (VDE), of the 2004 Best Teaching Award of the TUM EE Faculty Students Association, of the 3rd prize of the 1996 Munich Business Plan Contest.

Stefano Lucidi received the M.S. degree in electronic engineering from the University of Rome La Sapienza, Italy, in 1980. From 1982 to 1992 he was Researcher at the Istituto di Analisi e dei Sistemi e Informatica of the National Research Council of Italy. From September 1985 to May 1986 he was Honorary Fellow of the Mathematics Research Center of University of

Wisconsin, Madison, USA. From 1992 to 2000 he was Associate Professor of Operations Research of University of Rome La Sapienza. Since 2000 he has been Full Professor of Operations Research of the University of Rome La Sapienza. He teaches Operations Research and Global Optimization Methods in Engineering Management. His research interests are mainly focused on the study, definition and application of nonlinear optimization methods and algorithms. This research activity has produced 76 papers published in international journals and 20 papers published in international books.

Industrial participation

MunEDA GmbH (MUN) Founded in 2001 in Munich Germany, MunEDA provides leading EDA technology for circuit migration, analysis, modelling, and optimization for custom design. MunEDA's solutions are in industrial use by leading semiconductor companies in the areas of communication, computer, memories, automotive, and consumer electronics. MunEDA's tool suite WiCkeD is a comprehensive and powerful software tool suite for manual, semi- and full automatic analysis and yield optimization of analog, mixed signal and digital circuits. MunEDA has offices in Munich, Germany (Headquarter) and Sunnyvale, California, USA (MunEDA Inc.). MunEDA is represented by leading EDA distribution companies worldwide in USA, Japan, Korea, Taiwan, China, UK, Scandinavia, South America and others. MunEDA Tools are used today by numerous major semiconductor companies (IDMs, Fabless,Designhouses) for wireless, automotive, RF, Memory and DRAM applications, down to 20/14nm. MunEDA is working with customers on a daily basis on actual design problems in the mixed signal and RF world and has lot of experiences in analog design and the actual enhanced technology generations. To be able to solve all customer requirements in this arena, all needed actual EDA Flows for mixed signal design, algorithm and methodologies are installed and can be used.
Since company start MunEDA has participated in several national and European in German/European Funding R&D projects such as ANASTASIA+ (MEDEA) VeronA, (BMBF), Sigma65 (BMBF), SyEnA (BMBF), HONEY (MEDEA), RELY (CATRENE), THERMINATOR (FP7), SMAC (FP7), MANON (Marie-Curie). In MANON MUN works on the implementation of RSM models as State-of-the-Art basis of the project. During the project MUN will work on an SW demonstrator together with the industrial and academic research partners.

STMicroelectronics (ST) is one of the worlds largest semiconductor companies with net revenues of US$ 8.49 billion in 2012. Offering one of the industry's broadest product portfolios, ST serves customers across the spectrum of electronics applications with innovative semiconductor solutions by leveraging its vast array of technologies, design expertise and combination of intellectual property portfolio, strategic partnerships and manufacturing strength. ST focuses its product strategy on sense and power technologies, automotive products, and embedded-processing solutions. The Sense and Power segment encompasses MEMS and sensors, power discrete, and advanced analog products. The Automotive portfolio covers all key application areas from powertrain and safety to car body and infotainment. The Embedded Processing Solutions include microcontrollers, digital consumer and imaging products, application processors and digital ASICs. ST products are found everywhere microelectronics make a positive and innovative contribution to people's lives. The Company's world-class products and technologies serve to: deliver compelling multimedia experiences to consumers anytime, anywhere in the home, in the car, and on the go; increase energy efficiency all along the energy chain, from power generation to distribution and consumption; provide all aspects of data security and protection; and contribute to helping people live longer and better by enabling emerging healthcare and wellness applications. ST is among the world leaders in a broad range of segments, including semiconductors for industrial applications, inkjet printheads, MEMS (Micro-Electro-Mechanical Systems), MPEG decoders and smartcard chips, automotive integrated circuits, computer peripherals, and chips for wireless and mobile applications.ST has a strong focus on delivering solutions that reduce energy consumption at the point of use in domestic and industrial applications; all aspects of security and data protection; and a growing presence in the emerging advanced healthcare market. The group has approximately 48,000 employees, 12 main manufacturing sites, advanced research and development centers in 10 countries, and sales offices all around the world. Since its creation, ST has maintained an unwavering commitment to R&D. Almost one quarter of its employees work in R&D and product design and in 2012 the Company spent about 28% of its revenue in R&D. Among the industry's most innovative companies, ST owns about 16,000 patents, about 9,000 patent families and 515 new filings. The Company draws on a rich pool of chip fabrication technologies, including advanced FD-SOI (Fully Depleted Silicon-on-Insulator) CMOS (Complementary Metal Oxide Semiconductor), mixed-signal, analog and power processes, and is a partner in the International Semiconductor Development Alliance (ISDA) for the development of next-generation CMOS

technologies. To provide its customers with an independent, secure and cost-effective manufacturing machine, ST operates a worldwide network of front-end (wafer fabrication) and back-end (assembly and test and packaging) plants. From its inception, ST established a strong partnership culture and now has a worldwide network of strategic alliances with key customers, suppliers, competitors, and leading universities and research institutes around the world. In addition, ST plays a key role in Europe's advanced technology research programs. ST has established a worldwide network of strategic alliances, including product development with key customers, technology development with customers and other semiconductor manufacturers, and equipment- and CAD-development alliances with major suppliers. These industrial partnerships are complemented by a wide range of research programs conducted with leading universities and research institutes around the world, in addition to playing a key role in Europe's advanced technology research programs such as CATRENE (Cluster for Application and Technology Research in Europe on NanoElectronics), a successor to MEDEA+, and industry initiatives such as ENIAC (European Nanoelectronics Initiative) and ARTEMIS (Embedded Computing Systems Initiative).

Mini-Symposium on Robust Variable-Structure Approaches for Control and Estimation of Uncertain Dynamic Processes

Andreas Rauh and Luise Senkel [11] [12]

In recent years, numerous variable-structure approaches have been developed for control of nonlinear dynamic systems and for the model-based estimation of non-measurable states and parameters. These approaches typically make use of first-order as well as higher-order sliding mode techniques and related procedures. One of their main advantages is the inherent proof of asymptotic stability. This stability proof is either performed offline during the corresponding controller as well as estimator design or online by the real-time evaluation of a suitable candidate for a Lyapunov function.

The methodological framework for variable-structure control and estimation approaches is quite well developed in the case of systems, for which process models are accurately known. Nevertheless, research efforts are still necessary to make the corresponding procedures applicable when only worst-case bounds are available for specific parameters (e.g. due to non-negligible manufacturing tolerances). Moreover, significant stochastic disturbances (e.g. as a result of measurement noise) may act as further system inputs in such applications. To enhance robustness in such cases, it is possible to combine techniques which are for instance based on interval analysis, stochastic differential equations, or linear matrix inequalities with variable-structure approaches. Finally, the adequate consideration of both actuator and state constraints represents a challenging task that is currently intensively investigated.

This Minisymposium aims at presenting ongoing research activities in the field of robust variable-structure control and estimation. The scope equally consists in highlighting novel methodological aspects as well as in presenting the use of variable-structure techniques in industrial applications including their efficient (software) implementation on hardware for real-time control.

The contributions to this Minisymposium contain

- Design of sliding mode control strategies under state and actuator constraints
- Sliding mode techniques for state and parameter estimation

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- Interval analysis for verified stability analysis of finite-dimensional dynamic systems with bounded uncertainty
- Stability analysis for dynamic systems described by stochastic differential equations
- Lyapunov techniques for variable structure systems
- Novel techniques for stability analysis of linear systems based on linear matrix inequalities and on the computation of the roots of (interval) polynomials
- Numerical verification and experimental validation for industry-motivated applications in control of fuel cell systems, automotive applications and mechanics as well as mechatronics.

List of confirmed contributors

- *P. Leśniewski and A. Bartoszewicz (University of Lódź, Poland)*: **Reaching Law Based Control of Mechanical Systems with Velocity and Acceleration Constraints**
  In this paper we propose a discrete time sliding mode congestion controller for a single virtual circuit in connection-oriented communication networks. The circuit is characterized by the non-negligible propagation delay, the maximum link capacity and unknown, time-varying data loss rate. The proposed controller generates non-negative and limited transmission rates, ensures upper bounded queue length in the bottleneck link buffer and may guarantee full utilization of the link capacity. These favorable properties are obtained in spite of a priori unknown packet losses in the controlled virtual circuit. In order to ensure fast reaction to the unpredictable data loss and unknown changes of the available bandwidth, the controller employs the dead-beat sliding hyperplane. However, straightforward application of the dead-beat paradigm could lead to unacceptably big transmission rates. Therefore, the controller is designed using the concept of the reaching law, which helps to attenuate the excessive magnitude of control signal at the beginning of the transmission process. The proposed reaching law leads to the non-switching type sliding mode controller which is robust with respect to mismatched disturbance and modeling uncertainty. The results given in the paper are demonstrated analytically and verified in a simulation example.

- *A. Rauh, L. Senkel, H. Aschemann (University of Rostock, Germany)*: **Interval-Based Sliding Mode Control for High-Temperature Fuel Cells under Actuator Constraints**
  In previous work, different approaches have been derived by the authors for the reliable control of the thermal behavior of high-temperature fuel cell stacks under consideration of uncertain parameters and not a-priori known load variations. These control approaches comprise model-predictive, feedback linearizing, and sliding mode techniques. It was shown that both the predictive and sliding mode techniques can be applied successfully to system models with interval parameters.

  In contrast to the predictive control approach, physical state and actuator constraints cannot be handled directly within a classical sliding mode design for this type of application. However, the sliding mode-type control design provides an inherent stability proof, which is not directly available for the predictive technique. For these reasons, this contribution removes the before-mentioned drawback concerning the handling of constraints by a reformulation of the stability conditions resulting from the variable structure control design. This reformulation is based on a stability-preserving nonlinear gain adaptation scheme that is employed as soon as saturation limits are reached. For that purpose, actuator limits are treated as hard constraints that must not be exceeded under all circumstances. State limitations, however, are described by soft constraints. They are considered by corresponding weak penalty terms.

  In such a way, it becomes possible to adapt the gain value of the variable-structure control part as well as the parameters characterizing the sliding surface during system operation in real time. These adaptations directly lead to a modification of the system dynamics during the transient reaching phase. This phase describes the system dynamics as long as the operating conditions do not fully comply with those system states for which the sliding condition is fulfilled. Moreover, a suitable trajectory planning procedure is presented. It allows for the specification of desired changes in the system outputs between different stationary operating points, where again the effects of limited actuator ranges and state constraints are addressed in addition with bounded uncertainty in the parameters of the nonlinear dynamic system model. Representative numerical results, based on experimental data from a test rig at the Chair of Mechatronics at the University of

Rostock, are shown to conclude this contribution.

- *L. Senkel, A. Rauh, H. Aschemann (University of Rostock, Germany)*: **Experimental Validation of State and Parameter Estimation using Sliding-Mode Techniques with Bounded and Stochastic Uncertainty**
  Uncertainties - more precisely bounded and stochastic disturbances - play a major role in control and estimation tasks in general. Examples for bounded uncertainty are lack of knowledge about specific parameters and manufacturing tolerances. Moreover, stochastic disturbances have a very important impact on dynamic systems, especially in sensor measurements. These issues make it difficult to control a system such that robustness and stability are guaranteed especially if system parameters are not exactly known and system states cannot be measured with high accuracy due to process and measurement noise. The mathematical description of the considered system including the most important deterministic characteristics is essential for a combined state and parameter estimation. Therefore, a sliding mode observer that copes with uncertain parameters as well as with noisy measurements is proposed in this presentation. States and parameters are estimated in such a way that the error dynamics are stabilized. The advantages of the presented observer are robustness and stability based on the usage of suitable candidates for Lyapunov functions as it is usually done in existing sliding mode approaches. The differences to existing sliding mode observers are that, firstly, no restrictive matching conditions occur which, hence, lead to a more general applicability of the observer. Secondly, interval descriptions are used for uncertain states as well as parameters. Finally, modeling different kinds of nonlinearities that inevitably in uence the stability of the system - as for example friction, wear of mechanic components or remanence of a brake - can be included as stochastic disturbances.

  Considering interval arithmetic is in general useful if a system is affected by uncertainty that in uences the system dynamics in an significant way. Therefore, not only intervals for parameters but also for measurement uncertainty and errors of the estimated states can be taken into consideration. The number of calculated switching amplitudes of the presented observer is equal to the number of measurements. This enables an individual computation of the switching amplitudes for the estimation of states and parameters according to the evaluation of a Lyapunov function using the Itô differential operator

for stochastic processes. Moreover, Pontryagin's maximum principle is used for an optimal input design to improve the parameter estimation.

Simulation results show the practical applicability of this approach for estimating states and parameters. Numerical results of the parameter estimation using the sliding mode approach are compared with a least-squares parameter identification to point out the improved performance of the observer. For this comparison, experimental data from a test rig available at the Chair of Mechatronics at the University of Rostock are used.

- *H. Schulte, S. Georg (HTW Berlin, University of Applied Sciences, Germany)*: **Polytopic Formulation of Sliding Mode Observers for Fault Reconstruction: Comparison between the LPV and Takagi-Sugeno Model Approaches**
  This paper compares recently proposed fault reconstruction methods using sliding mode observers for a class of linear parameter varying (LPV) with Takagi-Sugeno systems. Both methods are an extension of a canonical form for sliding mode observer design, originally restricted to linear time invariant systems. The methods are compared analytically and by simulation. The underlying relation between them is exposed.

  In the last decades, there has been an explosion of interest in the use of sliding mode methods for fault detection, isolation (FDI) and fault reconstruction using the equivalent output injection signal. The fault reconstruction can be exploited for fault tolerant control (FTC) in the sense that sensor and actuator faults are corrected before the measurements are used for the controller or rather the control signal acts on the plant. Originally, the sliding mode method is based on linear time invariant (LTI) systems with unknown but bounded terms. An important extension to the sliding mode observer concept is to introduce a convex combination of LTI systems. The combination can be parameter-varying or state-varying with the constraint, that all output matrices are common. The parameter-varying concept is based on a class of LPV systems. In contrast, the state-varying sliding mode concept was first proposed in Gerland et al., where the observer is implemented within a Takagi-Sugeno (TS) model structure to account for system nonlinearities. Both approaches proposed extensions of the LTI scheme of sliding mode observer to a convex combination of LTI systems, which is a suitable compromise between a full nonlinear

design and the LTI framework.

In this paper, differences and similarities between these methods were discussed in detail. The efficiency of the methods is investigated using two benchmark problems, the inverted pendulum and an aircraft problem from the literature.

- *A. Rauh, L. Senkel, H. Aschemann (University of Rostock, Germany)*: **Computation of Confidence Regions in Reliable, Variable-Structure State and Parameter Estimation**
  Interval-based sliding mode controllers and estimators provide a possibility to stabilize the error dynamics despite not accurately known parameters and bounded measurement uncertainty. However, current implementations of both types of approaches are commonly characterized by the fact that they only provide point-valued estimates without any explicit computation of confidence intervals. Therefore, this contribution aims at developing fundamental techniques for an extension towards the computation of guaranteed confidence intervals.

  The corresponding procedure is based on the use of symbolic formula manipulation and interval arithmetic for the computation of those sets of state variables (and estimated states, respectively) that can be reached in a finite time horizon. For that purpose, the nonlinear system dynamics is embedded into a (quasi-) linear state-space representation with piecewise constant input signals for which the sets of reachable states can be computed by using Müller's theorem, or more generally, by exploiting the system property of cooperativity for linear parameter-varying finite-dimensional state equations. The necessary proof for cooperativity is performed by verified range computation procedures that rely on interval arithmetic software libraries. Basic building blocks of these procedures are presented for the use of the Matlab toolbox IntLab.

  After a summary of the before-mentioned fundamental procedures, extensions are presented which show how these techniques can by employed in a framework for designing sliding mode estimators. These estimators, extended by the use of interval arithmetic, determine the sets of state variables and parameters that are consistent with both a given dynamic system model and information about bounded measurement uncertainty.

  Finally, necessary extensions are highlighted which allow for an extension of the implementation in such a manner that the corresponding

estimation schemes can make use of interval arithmetic in real time. Numerical results for estimation tasks related to the longitudinal dynamics of a vehicle conclude this contribution.

Online Industrial Mathematics

Matti Heilio, Poul Hjorth, Seppo Pohjolainen, Elena Vázquez Cendón, Leonid Kalachev, Sergei Zuyev

The omnipresence of the internet, and the associated rise of web-supported education, network-based projects, distance learning, and Open On-line Coursework, is both a challenge and an magnificient opportunity for ECMI. In this minisymposium we will examine a number of recent experiences with long-distance and cross-institutional education in industrial mathematics.

The cutting edge knowledge in the art of mathematical technology is located in small nodes, research groups on applied mathematics and scientific computing. Web-technologies are a viable media for innovative processes and knowledge transfer. We will discuss the opportunities in organizing education in modelling and applied mathematics.

The minisymposium will end with a discussion forum where we attempt to focus on the pitfals and strengths that the technology has in store for industrial mathematics. We wish to forward a vision of a European e-learning portal in applied mathematics, including for instance a database reflecting the supply of special math courses within the ECMI network, relevant to industry and real life applications. The speakers and talks are listed below.

Speakers

- Matti Heilio, matti.heilio@lut.fi, Finland, Lappeenranta University of Technology
- Poul Hjorth, P.G.Hjorth@mat.dtu.dk, Denmark, Technical University of Denmark
- Seppo Pohjolainen, seppo.pohjolainen@tut.fi, Finland, Tampere University of Technology
- Elena Vázquez Cendón, elena.vazquez.cendon@usc.es, Spain, University of Santiago de Compostela
- Leonid Kalachev, KalachevL@mso.umt.edu, United States, University of Montana
- Sergei Zuyev, sergei.zuyev@chalmers.se, Sweden Chalmers, Gothenburg

Mini-Symposium on Simulation and Optimization of water and gas networks

Prof. Dr. Gerd Steinebach [13] [14] *Prof. Dr. Oliver Kolb* [15] [16] *Prof. Dr. Jens Lang* [17] [18]

Short description

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

Motivation/Relevance to ECMI

Energy efficiency is a major topic in todays industry. In order to operate large networks in an efficient way, simulation and optimization will become common tools in future. In the research project EWave (= energy efficiency in water supply networks) of the German Federal Ministry of Research and Technology a prototype management tool for a large water supply authority shall be developed. The proposed modelling and numerical methods are applicable to other flow networks in industry as well.

Confirmed speakers

- Andreas Pirsing, Siemens AG: *Business Potential for information technology applications in Water (Smart Water Grids)*
- Gerd Steinebach, University of Applied Sciences Bonn-Rhein-Sieg: *From river Rhine alarm model to water supply network simulation*

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[18]Phone: +49 (0)6151 16-2389 , E-Mail: lang@mathematik.tu-darmstadt.de

- Jens Lang, Technical University Darmstadt: *Adaptive Discretization for Unsteady Transport Systems on Networks*
- Tim Jax, University of Applied Sciences Bonn-Rhein-Sieg: *ROW methods adapted to network simulation*
- Raul Borsche, Technical University Kaiserslautern: *Higher Order Numerical Schemes on Networks*
- Oliver Kolb, University Mannheim: *Combination of Linear and Nonlinear Programming Techniques for Optimization Problems in Gas and Water Supply Networks*
- Tanja Clees, Fraunhofer SCAI: Simulation and statistical analysis of gas networks with MYNTS.

Industrial participation

One major partner of the EWave project is the Siemens AG.

Mini-Symposium on Mathematical methods in medical imaging

Adérito Araújo [19] *and Sílvia Barbeiro* [20] [21]

Short description

The symposium will gather researchers interested in developing and implementing mathematical methods in the field medical imaging and related areas. Among the techniques to be discussed, one can mention, for instance, segmentation, denoising, feature extraction, clustering and classification, and object recognition. The contributions are devoted to mathematical modelling and numerical simulation to present latest findings in both theory and applications and assess new challenges on the topic.

Motivation/Relevance to ECMI

Medical imaging applies different techniques to acquire human images for clinical purposes, including diagnosis, monitoring, and treatment guidance. As a multidisciplinary field, medical imaging requires the improvements in both fundamental science and engineering applications. Recent years have seen a tremendous progress in mathematical methods for image processing as well as in the development of powerful medical imaging systems, promoting the collaboration between mathematicians, physicists, engineers and clinicians.

This symposium endeavours to provide a forum for presenting and discussing new mathematical methods for solving problems in medical imaging, and attempts to establish a bridge between mathematical research and its applications in medicine.

Confirmed speakers

- Alberto Gambaruto (University of Lisbon, Portugal): http://www.math.ist.utl.pt/ agambar/
- Eduardo Cuesta (University of Valladolid, Spain): http://www.researchgate.net /profile/Eduardo_Cuesta/

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[20] silvia@mat.uc.pt

- Karol Mikula (Slovak University of Technology, Slovakia): http://www.math.sk/mikula/
- Pedro Serranho (Open University, Portugal): http://www2.uab.pt/ departamentos/DCT/detaildocente. php?doc=111
- Slvia Barbeiro (University of Coimbra, Portugal): http://www.mat.uc.pt/ silvia/
- Tobias Preusser (Fraunhofer MEVIS, Jacobs University Bremen, Germany):http://www.mevis-research.de/ tp/

Mini-Symposium on Mathematical Modelling of Drug Delivery

Dr Sean McGinty and Professor Sean McKee [22] [23]

Short description

Medical device companies spend tens of millions of euros annually developing novel and sophisticated drug delivery devices. In the majority of cases an empirical approach is adopted during the product development stage resulting in a great many experiments, often involving animals. It is not uncommon for projects to be abandoned after great expense due to unacceptable performance in laboratory or clinical trials. Mathematical modelling of drug delivery devices has the potential to not only reduce the number of costly experiments in product development, and identify products which are doomed to failure, but also to provide a better understanding of the underlying drug release mechanism(s) and drug redistribution in living tissue. This is of critical importance since an element of control is often required: if too much drug is delivered to the biological system then toxicity can arise and if too little drug reaches the affected area then it will not have the desired effect.

This symposium will bring together researchers from across Europe who are applying mathematical models and techniques, both analytical and numerical, to try to better understand drug delivery in living systems. The Symposium will provide a platform for new methodologies and ideas to be discussed. Since the modelling of drug delivery involves solving a mass transport problem where diffusion, dissolution, convection and binding often play important roles, it is anticipated that the techniques and ideas presented may well be complementary and applicable to a number of different drug delivery systems.

Motivation/Relevance to ECMI

We believe that the proposed mini-symposium is relevant to ECMI for several reasons. Firstly, the theme of mathematical modelling of drug delivery fits well within the conference theme of mathematical models in life science.

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Secondly, as outlined in the short description, the problem of modelling drug delivery is of real Industrial importance. Through our own work on the modelling of a cardiovascular device known as a drug-eluting stent, we have become aware of the lack of modelling undertaken by device manufacturers who have traditionally adopted empirical approaches to product development. We passionately believe that modelling should be the first consideration since it can not only reduce the number of costly and time consuming experiments (not to mention the associated ethical issues) but also it can provide useful insights into the important parameters in the system. This, in turn, can help in developing a device with optimal performance. Thus we believe that the proposed mini-symposium will highlight the role of mathematical modelling of drug delivery and provide the opportunity for useful exchanges and collaboration. This will only serve to expedite model development.

Confirmed speakers

The proposed programme includes talks from British, Irish, French, Italian and Portuguese researchers who are all actively engaged in mathematical modelling of drug delivery.

- Dr. Sean McGinty, Department of Mathematics and Statistics, University of Strathclyde, Glasgow, UK
- Dr. Martin Meere, Department of Applied Mathematics, NUI Galway, Republic of Ireland
- Dr. Giuseppe Pontrelli, Istituto per le Applicazioni del Calcolo, CNR, Rome, Italy
- Professor Abdul Barakat, Cardiovascular Cellular Engineering Laboratory, Ecole Polytechnique, Paris, France
- Professor Jose Augusto Ferreira, Department of Mathematics, University of Coimbra, Portugal.

Industrial Participation

While we are unable to confirm any Industrial participation at this stage, we would like to stress that much of the research of the confirmed speakers is

supported either directly or indirectly by Industry and is driven by clinical need.

European Study Groups with Industry

Hilary Ockendon

Author Keywords: Modelling, Study Groups, Industry

In the year when the 100th ESGI will be held, it is timely to assess the effectiveness of this popular mechanism for enabling the interaction of industry and academic mathematicians. In this minisymposium, five speakers will describe their own experience of Study groups. Some talks will give an overview of how Study Groups work in a particular country and others will describe one or two problems that have been successfully solved. We will highlight the unique strength of mathematics as a technology transfer tool, where the same mathematics may apply in very different application areas, and the unreasonable effectiveness of a relatively simple mathematical model. The final slot will be a discussion session where we will address the pros and cons of the Study Group concept.

Speakers (proposed)

- Andreas Muench, University of Oxford
- Stefka Dimova, Sofia University
- William Lee, Limerick University
- Poul Hjorth, DTU, Copenhagen
- Aderito Araujo, University of Coimbra

Mini-Symposium on High Performance Computational Finance

Binghuan Lin (Techila Technologies/TUT)
Álvaro Leitao Rodríguez (TU Delft)
José Pedro Silva (Bergische Universität Wuppertal)
Jinzhe Yang (SWIP)

This is a joint minisymposium of the 2 Marie Curie Initial Training Networks **STRIKE** Novel Methods in Computational Finance and **HPC-Finance** Training in Modern Quantitative Methods and High-Performance Computing for Finance.

Motivation/Relevance to ECMI

The motivation for this minisymposium is twofold: first to exchange and discuss current insights and ideas, and to lay groundwork for future collaborations of these two networks. Secondly, this minisymposium is organized by the doctoral fellows themselves and doing so they will train intensively their skills in organizing events.

Confirmed speakers

- José Pedro Silva (Bergische Universitt Wuppertal): *Model Order Reduction Techniques for Basket Option Pricing*
- Álvaro Leitao Rodríguez (TU Delft): *Modelling and Numerical Techniques for Credit Valuation Adjustment*
- Binghuan Lin (Techila Technologies/TUT): *Financial application of SMC and Distributed SMC*
- Jinzhe Yang (SWIP): *FPGA implementation of SMC and FPGA-CPU collaborate architecture.*

Mini-Symposium on Non-hydrostatic wave propagation with depth averaged equations: models and methods

A.I. Delis [24] *and M. Ricchiuto* [25]

Short description

This symposium aims at providing an overview of the main challenges related to the simulation of near shore free surface flows by means of depth averaged Boussinesq type equations. This is a domain with enormous impact in the field of near-shore engineering (design of harbours, coastal defence structures, etc.), offshore engineering (platforms design, pipelines, etc.), naval engineering (design of vessels with optimized properties), and environmental management (morphodynamic evolution, pollutant transport, etc.).

Numerical simulations are essential tools for any design activity in which water waves play a significant role. The mathematical challenges related to the construction of numerical models are many. This mini symposium aims at covering several of these challenges. The topics covered in the talks range from the choice of the form of the PDEs, to their dispersion optimisation, to their discretization with appropriate very high resolution numerical methods. Additional topics will include the numerical treatment of wave breaking and of moving shorelines, which are phenomena of paramount importance for the hydrodynamics in the near shore region.

Motivation/Relevance to ECMI

The mini-symposium is in line with one of the five main themes of the conference, namely *mathematical methods in environnement*, and combines challenging topics related both to the choice of the form of the PDEs involved, and of their high order numerical discretization.

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[25]Dr. M. Ricchiuto INRIA Bordeaux-Sud-Ouest 200 Avenue de la Vieille Tour 33405 Talence cedex - France email : Mario.Ricchiuto@inria.fr tel : +33 5 24 57 41 17 - fax : +33 5 24 57 40 38

Confirmed speakers

- C. Eskilsson (Chalmers University) and A. Engsig-Karup (Tech.nical University of Denmark): *Spectral/hp element Boussinesq models in the open-source nektar++ framework*
- J. Sainte Marie (CETMEF and Inria Team Ange): *A non-hydrostatic Saint-Venant system. Derivation and validation*
- F. Marche (Université de Montpellier), D. Lannes (ENS Paris) and P. Bonneton (EPOC Bordeaux): *A splitting approach for the Green-Naghdi equations*
- M. Kazolea, A.I. Delis and C. Synolakis (Technical University of Greece): *Wave propagation, breking and runup with a Boussinesq type model*
- S. Bellec, M. Colin, A. Filippini and M. Ricchiuto (Inria Team Bacchus): *Conservative and non-conservative variants of weakly nonlinear Boussinesq models: derivation and numerical assessment.*

Other proposed speakers: D. Adytia and E. van Groesen (University of Twente).

Mini-Symposium on Tailored-Mathematics for the Technical Textile Industry

Nicole Marheineke [26]

Short description

Spunbond, Meltblowing, Air-laying, Fluid-dynamical Sewing, Electro-spinning are just a number of the various manufacturing processes for technical textiles. In the focus of all these processes stand slender objects (oriented particles, elastic threads or viscous/viscoelastic jets) that move due mechanical, electromagnetic or aerodynamical forces and interact with each other, outer walls and/or surrounding turbulent flows. The efficient simulation and optimization of the processes requires tailored mathematical models and methods.

Motivation/Relevance to ECMI

ECMI aims to promote the application of mathematical models and methods in industry and to support academic collaborations on an international scale. Mastering the complexity of the production processes of technical textiles implies the sharing of different tools, which requires a high level of communication between different mathematical, physical and engineering schools. This minisymposium brings together expertise from asymptotics, stochastics, numerics and experiments. It provides an appropriate platform for discussions and promotes young researchers.

The practical relevance for industry is evident by the attendance of industrial partners and the contributions from Fraunhofer ITWM, Kaiserslautern. A special feature of the minisymposium are the so called *PracTheo double talks* jointly given by industrial and academic colleagues. Moreover, some of the research results are derived within the project OPAL *Optimization of Airlay-Processes* in collaboration with two leading companies of German technical textile industry. OPAL is supported by the German Federal Ministry for Education and Research in the program *Mathematics for Innovations in Industry and Service*.

Confirmed speakers

- **PracTheo double talk,** K. Becker (AUTEFA Solutions, Austria) and S. Gramsch (Fraunhofer ITWM, Germany)
- **PracTheo double talk,**J. Rivero (Sevilla, Spain) and W. Arne (Fraunhofer ITWM, Germany)
- B. Audoly (CNRS, Universite Paris 6, France), M. Wardetzky (U. Göttingen, Germany)
- S. Martin (Imperial College London, UK), L.L. Bonilla (Madrid, Spain), A. Klar (TU Kaiserslautern, Germany)
- C. Nessler, A. Klar (TU Kaiserslautern, Germany)
- S. Schiessl, N. Marheineke (FAU Erlangen-Nürnberg, Germany), R. Wegener (Fraunhofer ITWM, Germany)
- C. Strohmeyer, G. Leugering (EAM and FAU Erlangen-Nürnberg, Germany)
- E. Suli (Oxford, UK)
- A. Vibe and S. Strunk, N. Marheineke, E. Bänsch (FAU Erlangen-Nürnberg, Germany).

Mini-Symposium on a European Network of Mathematics for Industry and Innovation

Peregrina Quintela Estevez [27]
Antonino Sgalambro [28]

Organizer(s)-Institutions

- EU-Maths-IN — Stichting European Service Network of Mathematics for Industry and Innovation
- AMIES — Agence pour les mathématiques en interaction avec l'entreprise et la société. France
- KoMSO — Komitee für mathematische Modellierung, Simulation und Optimierung. Germany
- Math-in — Red Española Matemática-Industria (Spanish Network for Mathematics & Industry). Spain
- Smith Institute — Smith Institute for industrial mathematics and systems engineering. United Kingdom
- SM[i]^2 — Sportello Matematico per l'Industria Italiana (Mathematical desk for Italian Industry). Italy
- PWN — Platform Wiskunde Nederland. Netherlands

Short description

The development of new products or production processes today is dominated by the use of simulation and optimization methods that, based on a detailed mathematical modeling, support or even replace the costly production of prototypes and classical trial-and-error methods. To address this development and following the Recommendations of the Forward Look

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[28]SM[i]^2 - Sportello Matematico per l'Industria Italiana. Italy c/o Istituto per le Applicazioni del Calcolo *Mauro Picone* National Research Council of Italy email: a.sgalambro@iac.cnr.it tel: +39-06-49270970

Mathematics and Industry published by the European Science Foundation, several European research networks have established a new organization to increase the impact of mathematics on innovations in key technologies and to foster the development of new modeling, simulation and optimization tools.

In order to present the goals and strategies of EU-MATHS-IN and the operational background of its founding members, some mini-Symposia will be organized to collect and present the industrial experiences of these organizations in cooperation with their research partners, highlighting, when possible, the benefit for the interested firms.

The first session of mini symposium, entitled:

EU-MATHS-IN: a European network of networks in industrial mathematics

will be devoted to introduce the goals and strategies of the new European network, together with the organization and the role of each national node member of EU-MATHS-IN, including their legal organization, their way of working to promote the relationship between researchers and businesses, how they spread the skills and experience of their groups, how they act as a one stop shop for their groups, which research groups / entities are represented in the node or how to become a member. EU-MATHS-IN would have 30' for its presentation, while each member national networks will be presented in 15/20' by one of its representatives.

Then, three sessions of two hours will follow, entitled:

EU-MATHS-IN: European success stories with Industry

by collecting 2 contributions from each national network (12 short talks of 30' / 3 sessions). In particular, sessions could be organized by sorting the speeches with respect to the mathematics content, such as:

- Mathematical modeling, Applied and Stochastic Analysis;
- Numerical Analysis, Simulation and Scientific Computing;
- Optimization and Discrete Mathematics.

and/or on the base of the industrial sector they refer to.

Motivation/Relevance to ECMI

This network-of-networks named EU-MATHS-IN, sponsored by the European Mathematical Society EMS and the European Consortium for Mathematics in Industry ECMI, aims to become a dedicated one-stop-shop and

service unit to coordinate and facilitate the required exchanges in the field of application-driven mathematical research and its exploitation for innovations in industry, science and society.

The new organization has been established in Amsterdam on Nov. 27, 2013 with a joint meeting of the stakeholders: currently, six national networks are members of the EU-MATHS-IN foundation, and the number of members will increase as soon as new national networks in industrial mathematics will join the project.

In order to present the goals and strategies of EU-MATHS-IN and the operational background of its founding members, the mini-Symposia will be organized to collect and present the industrial experiences of these organizations in cooperation with their research partners, highlighting, when possible, the benefit for the interested firms.

Confirmed speakers

- Mario Primicerio, President of EU-MATHS-IN; Magnus Fontes, President of ECMI and its representative in the Executive Committee of EU-MATHS-IN; and a EMS representative in the Executive Committee of EU-MATHS-IN
- Georges-Henri Cottet AMIES (Agence pour les mathématiques en interaction avec l'entreprise et la société) France
- Hans-Georg Bock - KoMSO (Committee for Mathematical Modelling, Simulation and Optimisation) Germany
- Antonino Sgalambro SM[i]^2- Sportello Matematico per l'industria italiana Italy
- Peregrina Quintela Estevez - Math-in (Red espaola matemtica-industria) Spain
- Evgeny Verbitskiy - Platform Wiskunde Nederland - The Netherlands
- Robert Leese - The Smith Institute for industrial mathematics and System engineering UK.

Other proposed speakers. At least two researchers from each one of the six national networks will be among the speakers who will present two distinct success stories at the mini-symposia.

Industrial Participation

Whenever it will be possible, a representative from each company involved in the industrial success stories will be involved in the talks, together with the researchers, to expose the business benefits obtained by the firms.

Mini-Symposium on Simulation and Optimization of Solar Tower Power Plants

Martin Frank, Pascal Richter [29][30]

Short description

Solar tower power plants use many at mirrors to concentrate sun light on an absorber, which is mounted on a tower. The simulation of solar tower power plants plays an important role in the planning stage of a project. The goal is to find the most efficient arrangement of mirrors that balances power production against construction costs. The high computational cost associated with a sufficiently accurate simulation, and constraints on mirror positions, makes the optimization of a solar tower power plant a very challenging mathematical problem.

Motivation/Relevance to ECMI

The purpose of this mini-symposium is to report on the continuing progress of simulation and optimization strategies for solar tower power plants. It brings applied mathematicians together with engineers from the solar power community, and is designed specifically as a forum for researchers in earlier stages of their career to discuss their work and exchange ideas.

Confirmed speakers

- Paul Gauché, Solar Thermal Energy Research Group, Stellenbosch University, South Africa
- Fathia Eddhibi, Centre de Recherche et des Technologies de l'Energie, Borj Cdria, Tunesia
- Peter Schöttl, Fraunhofer Institute for Solar Energy Systems, Freiburg, Germany
- Pascal Richter, Mathematics (CCES), RWTH Aachen University, Germany

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Other proposed speakers

- Reiner Buck, German Aerospace Center (DLR), Stuttgart, Germany
- Alexander Mitsos, Process Engineering, RWTH Aachen University, Germany

Mini-Symposium on The intersection of theoretical and experimental industrial science

Dr. Ian Griffiths [31]

Overview

The Collaborative Workshop Initiative (CWI) is a new strategy for instigating collaboration between theoreticians and experimentalists to drive advances in industrial technological applications in areas where such complementary skills are essential. Organized by Dr Ian Griffiths, the CWI is entering its fourth year and has developed from a collaborative initiative between the University of Oxford's Mathematical Institute and Princeton University's Complex Fluids Group to an organization that now involves 18 global research institutions.

This mini-symposium aims to bring exposure to the CWI by presenting some of the successes of this initiative so far, to give a flavour of the meeting remit with the aim of expanding on the network that has been developed. The mini-symposium will focus on the following areas in which theoretical and experimental efforts have proven vital:

Membrane science and design: With interaction from world-leading industry Pall Corporation we have developed new tools for understanding the clogging, or *fouling*, of membranes from contaminants to inform the design of new water purification devices. New experimental techniques have revealed the potential to control fluid slip and hydrophobicity of membrane interfaces which may be useful in controlling their filtration efficacy.

Dynamics of snap-buckling: Snap-buckling refers to the response of an elastic beam or shell from a state of instability. Such devices may be used for biomedical valves, switchable optical devices, responsive hydrogels, and in aerospace engineering. Here a dynamic theory coupled with experimental validation provides the key ingredients to advance this scientific field.

Design of nuclear fusion reactors: Erosion and corrosion in water-cooled devices can have catastrophic implications. For instance in the ITER Project, an industrial feasibility study for nuclear fusion, the coolant systems must be able to last for the 30-year lifetime of the tokamak. Theory and experiment provide predictions for the requirements of the coolant system to ensure structural rigidity is maintained. Within the tokamak itself liquid

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metal is allowed to flow down the curved walls to transport heat from the central core. Understanding the development of Rayleigh Taylor instabilities in such fluids is key in determining the required thickness and flow speeds for effective heat transport.

Elastocapillary coalescence: microlithography is a burgeoning field with the continued efforts to reduce the size of microcomputers and other microelectromechanical systems (MEMS). The fact that surface tension can bend, and even break, microstructures is an important consideration in the etching process of MEMS fabrication. We present a theory with complementary experiments that gives insight into the behaviour and limitation of wet etching for MEMS fabrication.

Tentative list of speakers

- Dr Ian Griffiths, Oxford, U.K.
- Professor John Lister, Cambridge, U.K.
- Dr Derek Moulton, Oxford, U.K.
- Dr Guy Ramon, Technion, Israel
- Professor Peichun Amy Tsai, Twente, Netherlands
- Professor Stephen Wilson, Strathclyde, U.K.
- Dr Daniele Vigolo, ETH Zurich, Switzerland.

Other proposed speakers

- Reiner Buck, German Aerospace Center (DLR), Stuttgart, Germany
- Alexander Mitsos, Process Engineering, RWTH Aachen University, Germany

Minisymposium on Mathematical and numerical modeling of the cardiovascular system

Piero Colli Franzone, Luca F. Pavarino and Simone Scacchi

Author Keywords: Modelling, Study Groups, Industry

In the year when the 100th ESGI will be held, it is timely to assess the effectiveness of this popular mechanism for enabling the interaction of industry and academic mathematicians. In this minisymposium, five speakers will describe their own experience of Study groups. Some talks will give an overview of how Study Groups work in a particular country and others will describe one or two problems that have been successfully solved. We will highlight the unique strength of mathematics as a technology transfer tool, where the same mathematics may apply in very different application areas, and the unreasonable effectiveness of a relatively simple mathematical model. The final slot will be a discussion session where we will address the pros and cons of the Study Group concept.

Speakers

- Andreas Muench, University of Oxford
- Stefka Dimova, Sofia University
- William Lee, Limerick University
- Poul Hjorth, DTU, Copenhagen
- Aderito Araujo, University of Coimbra

Minisymposium proposal on Mathematics and CAGD: interactions and intersections

Costanza Conti and Lucia Romani

Author Keywords:drug development, pharmacology, dose optimization

In the drug development arena, the rapid accumulation of new quantitative methodologies and tools pushed the emergence of systemic and mechanistic studies of pharmacology that drive the drug R&D. Particularly, tools based on modeling and simulation (M&S) gained a large popularity in the milieu considering the increasing number of success stories involving M&S. The efficient use of these tools heavily relies on advanced mathematical methodologies and their appropriateness to the problem at hand. This minisymposium will exemplify this field with mathematical applications to concrete pharmaceutical problems. Motivation/Relevance to ECMI : new venues for applied mathematics, with a high interest from pharmaceutical industry

Speakers

- Fahima Nekka (fahima.nekka@umontreal.ca) Faculté de Pharmacie and CRM, Université de Montréal, Canada
- Jun Li (li@crm.umontreal.CA) CRM, Université de Montréal, Canada
- Matylda Jablonska-Sabuka (matylda.jablonska-sabuka@lut.fi) Lappeenranta University of Technology, Finland
- Marco Veneroni (marco.veneroni@unipv.it) Università degli Studi di Pavia, Italy

Minisymposium proposal on Mathematics and CAGD: interactions and intersections

Costanza Conti and Lucia Romani

Author Keywords: Computer Aided Geometric Design, Theoretical and applied issues, arising from technology and industry.

Motivation,short description, relevance to ECMI

Computer aided geometric design (CAGD) concerns itself with the mathematical description of shapes for use, for example, in computer graphics, manufacturing, CAD/CAM, scientific visualization, or computer animation. Drawing from many areas and influencing others, CAGD is inherently interdisciplinary involving geometry, computer graphics, numerical analysis, approximation theory, data structures, linear and computer algebra. CAGD started in the 1960s, going back to efforts by Citroen and Renault in France and by Boeing and General Motors in the U.S. The term Computer Aided Geometric Design was coined after the 1972 conference at the University of Utah, organized by R. Barnhill and R. Riesenfeld, and since then it became a discipline in its own right. In recent years the interest in CAGD and its applications is beyond the mentioned contexts, not only because graphical applications are spreading their diffusion and increasing their request in different fields (industrial, medical, biological, topographic, geological applications) but also as a consequence of the relevant theoretical problems originated in the field, which are considered stimulating not only in the "contiguous disciplines" of numerical analysis and geometry, but also in different contexts. Therefore, aim of this mini-symposium is to gather academic and industrial scientists to give notice of new mathematical methods for the description of geometric objects. In particular, the selected talks will deal with both theoretical and applied issues arising from technology and industry.

Organizers

- Costanza Conti, Università degli Studi Firenze, Dipartimento di Ingegneria Industriale, Viale Morgagni 40/44, Firenze, Italia
  tel: 055-4796713, costanza.conti@unifi.it

- Lucia Romani, Universitadègli Studi Milano-Bicocca, Dipartimento di Matematica e Applicazioni, Via R. Cozzi 55 Milano, Italia
  tel: 02-64485735, lucia.romani@unimib.it

Speakers

- Hartmut Prautzsch, Karlsruhe Institute for Technology, Germany
- Weiyin Ma, Department of Mechanical and Biomedical Engineering, City University of Hong Kong, China
- Tomas Sauer, FORWISS (Institute for Software Systems in Technical Applications of Computer Science `http://www.forwiss.uni-passau.de`), Passau, Germany
- Christian Arber, TOPSOLIDE (`http://www.topsolid.fr/`), Paris, France,

Shape and Size in Biomedicine, Industry and Materials Science: an ECMI Special Interest Group

Alessandra Micheletti

Author Keywords: Stochastic Geometry, Statistical shape analysis, Mathematical morphology, Material Sciences, Industrial Applications

This is a minisymposium of an ECMI Special Interest Group which originated about 12 years ago from a working group of the Network of Excellence MACSInet and is now continuing its activities with the support of ECMI. A web page with a description of the activities of the ECMI-SIG can be found at

`http://www.mat.unimi.it/users/shape/.`

Statistical Shape Analysis and Stochastic Geometry deal with the geometrical information of families of objects in presence of stochasticity. Thanks to the development of information technologies, the last decades have seen a considerable growth of interest in the statistical theory of shape and its application to many and diverse scientific areas. Often the diagnosis of a pathology, or the description of a biological process mainly depend on the shapes present in images of cells, organs, biological systems, etc., and mathematical models which relate the main features of these shapes with the correct outcome of the diagnosis, or with the main kinetic parameters are often still not present. In material sciences, and industrial applications optimization for quality control requires mathematical models from Stochastic Geometry and the related statistical estimation procedures, and methods of Statistical Shape Analysis for comparison of different random geometrical patterns. From the mathematical point of view, Shape Analysis and Stochastic Geometry use a variety of mathematical tools from differential geometry, geometric measure theory, stochastic processes, etc., dealing with both direct and inverse problems. As far as applications are concerned, in this minisymposium topics which are relevant in biomedicine and material sciences will be emphasized.

Speakers

- A. Pietrasanta, D. Jeulin, F. Willot (CMM, Mines ParisTech); F. Moreau, L. Sorbier, M. Moreaud (IFPEN, Solaize), Mathematical Morphology of mesoporous alumina: design of a 3D random set model from TEM micrographs

- K. Losch, C. Redenbach (TU Kaisersalutern) Modelling of composite materials including complexly shaped particles
- S. Zuyev (Chalmers University) TBA
- A. Micheletti (Università degli Studi di Milano) Stochastic simulation and mathematical morphology for dual phase steel formation

Success stories from the ECMI Educational Programme

José Maria Gambi Fernandez and Alessandra Micheletti

Author Keywords: Education, Industrial Mathematics, Success Stories

Abstract

The ECMI Educational Programme in Mathematics for Industry started in 1987 and evolved in time, according to the increasing new requirments coming both from the industrial and academic world. Its basic ingredients anyway remained the same during the evolutions, and could be summarized in the following items:

- stimulating interdisciplinarity and team working of students
- training students in mathematical modelling
- encouraging students mobility in Europe.

The programme is now running since 25 years and its success is proven by the large number of former ECMI students who had success in their professional life, also thanks to the education that they received. In this minisymposium some *success stories* of former ECMI students will be presented, also to encourage new European centers to join the Consortium and set up and run the ECMI Educational Programme in their countries/regions.

Speakers

- Nicole Marheineke, University of Erlangen-Nürnberg
- Filippo Terragni, University Carlos III Madrid
- Alessandra Micheletti, Università degli Studi di Milano
- Eddie Wilson, University of Bristol

Mini-symposium: FEniCS and dolfin-adjoint: Innovative tools for automated finite element simulations

Steven Vandekerckhove and Garth Wells

Author Keywords: Partial Differential Equations, Finite Element Simulations, Adjoint Problems, High Performance Computing, Multi-Physics, Cut Meshes, Perfectly Matched Layer

Abstract

Partial Differential Equations (PDEs) are one of the most frequently used mathematical models for physical problems. It is often extremely hard to analytically solve these equations for technically relevant problems. Hence these problems are solved with numerical techniques. Often finite difference methods are applied, but they fail to approximate complicated geometries. Finite element (FE) methods allow unstructured meshes to overcome this problem, but have the disadvantage of a significant higher implementation cost.

The FEniCS Project is a collaborative project for the development of innovative concepts and tools for automated scientific computing, with a particular focus on automated solution of differential equations by FE methods. FEniCS permits dramatic gains in modelling productivity. This mini-symposium discusses several applications that benefit greatly from the FEniCS project.

First, we consider multi-domain and multi-physics problems with moving interfaces and parameter studies with changing geometric domains. These can be severely limited by the use of conforming meshes. To overcome these limitations, we focus on recent FE methods on cut meshes (CutFEM). CutFEM technologies allow flexible representations of complex or rapidly changing geometries by decomposing the computational domain into several, possibly overlapping domains. We explain how sophisticated computational geometry methods combined with the FEniCS tool chain for automated solution of PDEs gives an efficient and easy-to-use framework for implementing schemes based on overlapping meshes and non-matching interfaces.

The second application under consideration is the simulation of large problems involving turbulent flow and deformation of solids in fluid-structure interactions. To be able to resolve the scales of interest we use adaptive

FE methods. Efficient parallelization of the FEniCS FE-core DOLFIN was necessary to solve this problem. We will present the basic algorithms and applications which show the scalability and robustness of the parallelized version of DOLFIN.

Next we consider optimization problems constrained by PDEs. To solve these problems, Newton's method is widely considered to be the gold standard. The key ingredients required for Newton's method are fast gradient evaluations and fast Hessian actions. We discuss how the dolfin-adjoint software system may be used to automatically compute gradients and Hessians of functionals of PDE solvers written using FEniCS, even those of complex coupled nonlinear time-dependent equations, via the automated derivation and solution of the associated adjoint, tangent linear and second-order adjoint equations. The presented techniques rely on the automated transformation of a symbolic representation of the variational structure of the forward problem, as explicitly available in the Unified Form Language (UFL) format employed by FEniCS.

Finally, we consider wave propagation problems that require the truncation of infinite domains, in order to be able to use finite meshes for numerical simulations. In 1994 Berenger proposed the use of Perfectly Matched Layers (PMLs) for solving electromagnetic problems simulated with finite difference time domain methods. In 1996 Chew and Jin proved that, for this case, second order polynomial attenuation functions are optimal, and suggested that these results also were to be expected for FE methods, but lacked the means to test this hypothesis. The combination of FEniCS and dolfin-adjoint is however able to finally tackle this problem.

This mini-symposium aims to bring together researchers from engineering, applied mathematics and numerical analysis who are developing, analysing, optimizing or using finite element methods.

Relevance to ECMI

Partial differential equations are widely used in many real life applications. Having a powerful open-source tool and community to rapidly enlarge the set of feasible problems, has already proven valuable for applications in, e.g., aeronautics and non-destructive testing.

Speakers (confirmed)

- Andre Massing, Simula Research Laboratory

- Bärbel Janssen, KTH Royal Institute of Technology
- Patrick Farrell, University of Oxford / Christ Church College Oxford
- Steven Vandekerckhove, KU Leuven

Proposed (additional) speakers

- Garth N. Wells, University of Cambridge
- Jesus College Cambridge - Martin Alnaes, Simula Research Laboratory

Mini-Symposium on Semiclassical and quantum transport in semiconductors and low dimensional materials

M. Alvaro, L. Bonilla [32]*, O. Muscato, V. Romano* [33]

Description/Relevance to ECMI

Appropriate descriptions of electron transport in semiconductor micro and nano devices are crucial for many current and future technologies able to generate great industrial and economic activity. This minisymposium will explore a wide variety of topics in modern electron transport including numerical and stochastic methods for electron transport equations, thermal effects, sub-band models, quantum dots, wires, wells and superlattices, and semiclassical and quantum transport in graphene and carbon nanotubes

Tentative list of speakers

- M. Alvaro (Madrid)
- L. Barletti (Florence)
- L. Bonilla (Madrid)
- V. D. Camiola (Pisa)
- M. Carretero (Madrid)
- C. de Falco (Milano)
- A. Majorana (Catania)
- O. Morandi (Strassburg)
- O. Muscato (Catania)
- G. Platero (Madrid)

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[33]Dipartimento di Matematica e Informatica, Università di Catania, 95125 Catania, Italy

- V. Romano (Catania)
- F. Vecil (Granada).

Mini-Symposium on Parameterized model order reduction methods for complex multidimensional systems

Francesco Ferranti [34]
Wil Schilders [35]

Short description

This mini-symposium will focus on Parameterized Model Order Reduction (PMOR) methods for complex multidimensional systems. In recent years, PMOR methods have attracted a lot of attention from several scientific and industrial communities (e.g. electrical, chemical, biomedical engineering) as a powerful tool to significantly speed-up analysis and design of complex systems. Several analysis and design activities, such as design optimization, sensitivity and variability analysis, require multiple simulations of the system behavior for multiple values of the design parameters (e.g. layout features of an electronic system). Using physics-based solvers (e.g. electromagnetic solvers to solve Maxwell's equations, fluid dynamic solvers to solve Navier-Stokes equations) for these tasks becomes very computationally expensive. PMOR methods are advanced modeling and mathematical tools that allow to greatly reduce the computational cost of crucial analysis and design activities, without compromising the accuracy of the results.

The talks of the proposed mini-symposium will discuss state-of-the-art PMOR methods in different domains: chemical processes, nonlinear electronic systems, fluid dynamic systems, delayed differential systems.

Motivation/Relevance to ECMI

The proposed mini-symposium perfectly fits the aim and scope of ECMI 2014. PMOR methods are modeling and mathematical tools that can be used and applied to multiple research and industrial domains (e.g. electrical, chemical, biomedical systems). To give a practical example, in recent

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years the demand of the electronics industry for mathematical methods used in electronic design automation (EDA) software has witnessed a tremendous growth. Most current EDA methods and the tools that support them are inadequate for the design of modern complex systems, for which they must take into account an enormous number of design specifications and parameters: e.g. process, voltage and temperature (PVT) variation, power consumption, process constraints and yield requirements. Therefore, PMOR methods become imperative to address present-day challenges in the electronics industry.

Confirmed speakers

- Prof. Luca Daniel, Department of Electrical Engineering and Computer Science, Massachusetts Institute of Technology (MIT)
- Dr. Pascal Bolcato, Engineering Manager of analog simulators at Mentor Graphics
- Dr. Yao Yue, Computational Methods in Systems and Control Theory research group, Max Planck Institute for Dynamics of Complex Technical Systems
- Dr. Francesco Ferranti, Department of Information Technology, Ghent University - iMinds

Other proposed speakers

- Dr. Gianluigi Rozza, SISSA, International School for Advanced Studies, MathLab *Innovating with Mathematics*

Industrial participation

Dr. Pascal Bolcato from Mentor Graphics will be a speaker of the minisymposium. Dr. Bolcato has several patents under his name, mainly on analog and radio frequency signal simulator environments. Mentor Graphics is a leader company in EDA software. Dr. Bolcato will give a talk on the use of PCells (parameterized cells) in EDA softwares. The PCell concept is a recent and very important development in the EDA industry.

Model reduction in Continuum Thermodynamics

Eduard Feireisl, Josef Malek, Vit Prusa and Petr Schill

Author Keywords: modeling of complex materials, continuum theory of interacting continua, mathematical analysis of complete problems, model reduction, computer simulations.

Abstract

The purpose of the minisymposium is to present several approaches that illustrate how the complicated system of PDEs describing complex heat-conducting flows of multicomponent or rheologically complicated materials can be reduced to a simplified system that can be used in solving problems connected with real world applications (particularly focused on glass float technology, flows of fluids with pressure dependent viscosity in journal bearings, deformation of asphalt). The link connecting modelling issues, rigorous mathematical analysis and computer simulations focused on specific applications will be emphasized.

Organizers: Eduard Feireisl and Josef Malek.

Speakers (confirmed)

- Eduard Feireisl (Institute of Mathematics, Academy of Sciences, Prague, Czech Republic);
- Vit Prusa (Mathematical Institute, Charles University in Prague, Czech republic);
- Josef Malek (Mathematical Institute, Charles University in Prague, Czech republic);
- Petr Schill (Glass Service, Vsetin, Czech Republic).

Mini-Symposium on Selected Topics in Semi-Classical and Quantum Transport Modeling

Dragica Vasileska [36] [37]

Short description

The purpose of this mini-symposia is to bring together scientists from all over the world to discuss modeling of devices of present and future interest to both academia and industry.

Motivation/Relevance to ECMI

Computational electronics is a multidisciplinary field which encompasses disciplines such as physics, mathematics, electrical engineering, material science, etc. and has significant relevance to industry as simulation helps in the development process and shortens the time to market of the products.

Confirmed speakers

- Massimo Fischetti, University of Texas at Dallas, TX, USA
- Victor Sverdlov, Technical University of Vienna, Austria
- Mihail Nedjalkov, Technical University of Vienna, Austria
- Salvatore Amoroso, University of Glasgow, United Kingdom
- Zlatan Stanojevic, IUE, Technical University of Vienna, Austria
- Neophitus Neophitu, University of Warwick, United Kingdom
- Clemens Heitzinger, Arizona State University, Tempe, AZ, USA
- Philippe Dollfus, University Paris Sud, France
- Eric Pop, Stanford University, CA, USA
- Katerina Raleva. UKIM, Skopje, Republic of Macedonia.

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Other proposed speakers

- David K. Ferry, Arizona State University, Tempe, AZ, USA
- Ivan Dimov, Bulgarian Academy of Sciences, Sofia, Bulgaria
- Christian Ringhofer, Arizona State University, Tempe, AZ, USA
- Eric Polizzi, University of Massachusetts, Amherst, MA, USA
- Yiming Li, NTCU, Taiwan
- Shela Aboud, Stanford University, CA, USA.

Industrial participation

- Ben Kaczer, IMAC, Belgium
- Olin Harteen, Freescale, USA.

Simulation, Model Order Reduction and Robust Optimization for Industrial E-Mobility Applications

Andreas Bartel and Sebastian Schöps

Author Keywords:coupled systems PDAEs, multiphysics, uncertainty Quantification, model order reduction, optimization, magnetoquasistatics

Abstract

This minisymposium addresses mathematical problems and new methods for the robust design of key components in E-mobility. These key components are for instance: electrical machines, batteries etc.

In the overall, multi-physical phenomena have to be modeled. This yields large systems of coupled partial differential algebraic equations. Enhancing these devices, one will also need to further approach their limits. Therefore the uncertainties of parameters needs to be included.

In the end, these systems have to be solved accurately and repeatedly (for uncertainty or for optimization). Thus besides modeling, efficient techniques for multi-physical simulation, optimization using reduced order models and uncertainty computations are in our focus.

Mathematicians and electrical engineers report about their joint work within the project SIMUROM funded by the German Federal Ministry of Education and Research in the framework *Mathematics for Innovation in Industry and Services*.

Planed Speakers with co-authors

- Oliver Lass, Stefan Ulbrich
- Alessandro Alla, Michael Hinze
- Zeger Bontinck, Sebastian Schps, Herbert De Gersem
- Kai Gausling, Andreas Bartel

Relevance for ECMI

The enhancement of the simulation and optimization of designs in the field of E-mobility is important for industry. With the help of our industrial

project partners, Robert Bosch GmbH and CST AG, we tackle industrial relevant problems.

Mini-Symposium on Structured Numerical Linear Algebra in Imaging and Monument conservation

Marco Donatelli and Stefano Serra-Capizzano [38] [39]

Short description

The proposed mini-symposium lies in the frontier between numerical methods in structured linear algebra/matrix theory and relevant applications in the restoration of blurred and noisy images (2D, 3D) and in the modeling of the monument degradation under the action of pollutants (e.g. of biochemical type). In reality, several tools from structured matrix-theory are ready to be used in this context, with the effect of substantial improvements in the computational efficiency and in the precision of the results. Conversely, new specific examples of applications pose new challenging mathematical problems to people working on numerical methods and in structured matrix theory.

The invited speakers have a remarkable experience in the numerical field and in the modeling of the two topics considered in the proposal: such researches indeed require multi-level techniques in order to deal with edges/details present in images and monuments and often the convergence of these techniques is well understood if the spectral properties (eigenvalue localization, eigenvalue distribution, asymptotic behavior, eigenvector character in terms of frequencies etc.) of the underlying structures arising from the approximation of the involved integral and differential operators. We recall that the approximation of integral equations in imaging leads to matrix-structures which are ill conditioned in the high frequency domain, while elliptic/parabolic partial differential equations, also of nonlinear and degenerate type, arise in both problems.

Motivation/Relevance to ECMI

We strongly believe that such themes are of great relevance to ECMI, because the considered problems arise in a wide variety of industrial applications including medical/astronomical/geological imaging and in the important theme of the conservation of the cultural heritage, which is crucial in all Europe and especially in countries as Italy.

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Confirmed speakers

6 people among the following:

- Thomas Huckle
- Alessandro Buccini
- Claudio Estatico
- Jim Nagy
- Lothar Reichel For Monument Conservation
- Matteo Semplice
- Roberto Natalini
- Armando Coco
- Stefano Serra-Capizzano

Other proposed speakers: see the list above

Industrial participation

Territorial Partners in Como (Comune di Como, Camera di Commercio)

Mathematical Problems from Semiconductor Industry

Giuseppe Alì and Giovanni Mascali

Affiliation and Contact Organizers

Giuseppe Alì, Università della Calabria, Dipartimento di Fisica, giuseppe.ali@unical.it
Giovanni Mascali, Universit della Calabria, Dipartimento di Matematica ed Informatica, g.mascali@unical.it

Short Description

The minisymposium will collect contributions related to problems arising in the context of coupled modeling, simulation and optimization in micro and nano-electronics.

Motivation/Relevance to ECMI

The minisymposium will collect contributions related to problems arising in the context of coupled modeling, simulation and optimization in micro and nano-electronics.

Confirmed speakers

- G. Alì
- F. La Via
- G. Mascali
- Yue-Ju Peng
- F. Vecil

Other proposed speakers: L. Barletti, L. Bonilla C. de Falco, G. Frosali, A. Juengel, S. Micheletti, O. Morandi, R. Sacco, and others

Industrial participation

Reseachers from ST-Microelectronics

Mini-Symposium on Numerical Methods in Volcano Geophysics

Gilda Currenti
Eugenio Sansosti

Affiliation and Contact Information of the Organizers

Gilda Currenti, Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Catania, Osservatorio Etneo, gilda.currenti@ct.ingv.it

Eugenio Sansosti, Istituto per il Rilevamento Elettromagnetico dellAmbiente, CNR, sansosti.e@irea.cnr.it

Short description

Volcanology is being evolved through quantitative approaches employed to investigate volcanoes, understand their dynamics, and forecast their hazards. The increasing use of remote sensing technologies has enhanced our ability to detect and track different volcanic processes accompanying the ascent of magma from source to surface, including hydrothermal activity, magma intrusion, conduit flow dynamics, pyroclastic flows and ash dispersal. The purpose of the mini-symposium is to present the state-of-the-art in the modeling-based assessment of satellite remote sensing observations applied to open questions and problems in volcano geophysics. The mini-symposium will address themes with specialists presenting the theory and implementation of various numerical approaches applied to advance our knowledge of volcanic processes and quantitatively assess the volcanic hazards.

Motivation/Relevance to ECMI

In proposing the ECMI Minisymposium *Numerical Methods in Volcano Geophysics*, our motivation is to bring geophysics and volcanology problems into focus and highlight the complexity in modelling the involved processes. Mathematical sciences play a central role in the effort to solve several challenges posed in volcano geophysics both at the modeling and computational level. We believe that the mini-symposium is of interest for ECMI for two

main reasons. The first one is that some of the models and methods developed in this context can be applied to similar problems in environmental and industrial contexts, and the second one consists in the possibility of importing ideas from other fields in which similar issues have been addressed. We aim to attract interest among the applied mathematics community, which could provide interesting new insights and ideas to afford problem in volcano geophysics.

Confirmed speakers

- Armando Coco, Gilda Currenti, Ciro Del Negro, Giovanni Russo, University of Catania: A Second Order Finite-Difference Ghost-Point Method for Elasticity Problems on unbounded domains with applications to Volcanology;
- Sébastien Court, Olivier Bodart, Jonas Koko, Valérie Cayol, Université Blaise Pascal: Fictitious domain methods for fracture models in elasticity;
- Giuseppe Petrone, BE CAE & Test: Numerical models for volcano geothermal resources
- Carlino S., Troiano A., Di Giuseppe M.G., Somma R., Troise C., De Natale G., INGV-OV: Numerical modelling applied to Caldera unrest: the example of Campi Flegrei (Southern Italy)
- Antonio G. Camacho, Flavio Cannavò, Danila Scandura, Pablo J. González, Mario Mattia, and José Fernández, Instituto de Geociencias (CSIC-UCM), Facultad de Ciencias Matematicas: Study of magmatic intrusions in real time via ground deformation modeling: Application to 2008 Etna eruption
- Tim Masterlark, Ted Donovan, Kurt Feigl, Matt Haney, Cliff Thurber, Sui Tung, South Dakota School of Mines: Integrating seismic tomography with geodetic data to estimate volcano deformation sources.

Other proposed speakers

- Adelina Geyer, Institute of Earth Sciences *Jaume Almera* (CSIC) (Spain): ageyertraver@gmail.com

- Arnau Folch, Barcelona Supercomputing Center (Spain): arnau.folch@bsc.es
- Tim Wrigth, University of Leeds (UK): t.j.wright@leeds.ac.uk
- Thomas Walter, GFZ (Germany): twalter@gfz-potsdam.de
- Andrew Hooper, University of Leeds (UK): a.hooper@leeds.ac.uk

Industrial participation

BE CAE & Test (Giuseppe Petrone): giuseppe.petrone@be-caetest.it, gpetrone@diim.unict.it

Mini-Symposium on New progress on numerical modeling of Geophysical flows for environment, natural hazards, and risk evaluation

Manuel J. Castro Díaz,[40]
Carlos Parés Madroñal [41]
and Giovanni Russo. [42]

Short description

It is undisputed that the numerical simulation of geophysical processes plays nowadays a central role for understanding the interactions of complex natural phenomena and for making predictions when systems are perturbed. Moreover, in many cases, numerical models play an important role in the design of early warning system for natural disasters like tsunami or storm/hurricane alert systems.

The main goal of the mini-symposium will be the discussion and presentation of state-of-the-art computational and numerical methods for the next generation of geophysical flow models for environment, natural hazards, and risk evaluation with a focus on finite volume discretizations and HPC techniques for faster than real time simulations.

Motivation/Relevance to ECMI

This minisymposium fits in one of the specific topics of the Congress: 'Mathematical methods in envirnonment'. Mathematical models for environment, natural hazards, and risk evaluations are useful tools for public and private companies in different fields such as civil protection, hydraulic engeenering, assurances, etc. Therefore, the thematic of this minisymposium also fits in one of the main goals of ECMI: to promote the the use of mathematical models in activities of social or enconomic importance.

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Confirmed speakers

- Enrique D. Fernandez Nieto. Univ. de Sevilla
- Tomás Morales de Luna. Univ. de Cordoba
- Josá Manuel González Vida. Univ. de Málaga
- Michael Dumbser, University of Trento. (Italy)
- Alessandro Valiani, University of Ferrara (Italy)
- Edie Miglio, Politecnico di Milano (Italy)
- Alexander Kurganov, Tulane University, LA
- Alina Chertock, North Carolina State University, NC
- Christophe Berthon, Universit de Nantes (France)
- Jaques Sainte-Marie. UPCM-Paris 6 (France).

High Order One-Step ALE and AMR Methods for Conservative and Non-Conservative Hyperbolic PDE

Michael Dumbser

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Short description

In this talk we present a unified family of high order accurate finite volume and discontinuous Galerkin finite element schemes on moving unstructured and space-time adaptive Cartesian meshes for the solution of conservative and non-conservative hyperbolic partial differential equations.

The $P_N P_M$ approach adopted here uses piecewise polynomials u_h of degree N to represent the data in each cell. For the computation of fluxes and source terms, another set of piecewise polynomials w_h of degree $M \geq N$ is used, which is computed from the underlying polynomials uh using a reconstruction or recovery operator. The $P_N P_M$ method contains classical high order finite volume schemes ($N = 0$) and high order discontinuous Galerkin (DG) finite element methods ($N = M$) as two special cases of a more general class of numerical schemes. The schemes are derived in general ALE form so that Eulerian schemes on fixed meshes and Lagrangian schemes on moving meshes can be recovered as special cases of the ALE formulation. Furthermore, the method can also be naturally implemented on space-time adaptive Cartesian grids (AMR), together with time-accurate local time stepping (LTS). To assure the robustness of the method at discontinuities, a nonlinear WENO reconstruction is performed. The time integration is carried out in one single step using a high order accurate local space-time Galerkin predictor that is also able to deal with stiff source terms.

Applications are shown for the compressible Euler and Navier-Stokes equations, for the MHD equations and for the Baer-Nunziato model of compressible multi-phase flows.

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6. M. Dumbser, O. Zanotti, A. Hidalgo and D.S. Balsara. ADER-WENO Finite Volume Schemes with Space-Time Adaptive Mesh Refinement, *Journal of Computational Physics*, 248:257-286, 2013.

Mini-Symposium on Recent trends in modeling, analysis, and simulation of induction heat treatments

Dietmar Hömberg [43]
and Thomas Petzold. [44] [45]

Short description

Surface hardening is a well known method for enhancing the mechanical and tribological properties of components made of steel. This originates from the compressive residual stress which is generated by the occurring phase transitions in the boundary layer of the component.

The benefit of using electromagnetic induction for surface hardening in comparison to other heating technologies is that the heating energy is provided directly inside the boundary layer of the workpiece. This is advantageous with regard to energy consumption and allows a direct integration into the process chain.

In practice there is a need for a lot of pre-experiments for proper adjustment of a set-up for induction hardening of a newly designed component or when using a different material. With the improvement of computer technology and the use of finite-element methods the simulation of the process became of great interest for industry to avoid costly and time consuming experiments.

From a mathematical point of view, induction hardening phenomena can be modeled by a coupled systems of nonlinear partial differential equations comprising of Maxwell's equations and the heat equation together with the balance of momentum to compute mechanical strains and stresses arising from volumetric expansion during the phase transitions.

The minisymposium discusses new developments and results in the mathematical modeling, analysis and numerical simulation of induction hardening phenomena.

Motivation/Relevance to ECMI

The minisymposium presents new mathematical and numerical results for an important industrial process. All the talks are related to direct collaborations between math and industry.

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Confirmed speakers

- Pierre-Etienne Druet, Weierstrass Institute Berlin
- Francisco Ortegon Gallego, Universidad de Cadiz
- Thomas Petzold, Weierstrass Institute Berlin
- Alfred Schmidt, Universität Bremen.

Mini-Symposium on Simulation and control of hot-rolling

Dietmar Hömberg [46]
and Masahiro Yamamoto. [47]

Short description

Despite the development of sophisticated composite materials in recent years, steel is still the basic construction material for industrial societies. The development of new steels in the last decade has mostly been triggered by the demands of automotive industry to produce steel-intensive, safe, affordable, and fuel-efficient cars. Besides the development of new structural components such as tailored blanks and tubes, the main part of the innovations came from a consequential employment of modern multi-phase steels. These steels have shown high potential for automotive applications due to their remarkable properties combining high strength and good formability.

The standard process route for the production of multi-phase steel is by hot rolling and subsequent controlled cooling. It provides good microstructure homogeneity with acceptable surface quality for many applications.

The hot rolling process of dual phase (DP) steel consists of 4 steps:

- Rolling in roughing and finishing stands, which results in the refinement of austenite grain size due to the repeating static recrystallisation,
- Laminar cooling into two phase region
- Isothermal holding at ferrite transformation region temperatures, where the temperatures remain relatively constant,
- Fast continuous cooling to the required coiling temperature, during which martensite transformation takes place and bainite transformation can be avoided.

The biggest challenge in producing DP steel in this way is that the process window is very tight as only very short time in order of less than 10 s is allowed on the run out table according to its limited length.

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The goal of this minisymposium is to discuss various aspects of hot-rolling, where modern mathematical tools play an important role for an optimal configuration and process control of hot-rolling.

Topics to be addressed include recent developments in nucleation and growth models for the occurring austenite - ferrite phase transition, model reduction techniques for the efficient and accurate simulation of thermo-mechanical contact models to describe the rolling process, as well as second order optimal control strategies for the computation of optimal cooling strategies on the run-out table.

Motivation/Relevance to ECMI

The minisymposium presents new mathematical results for the modeling, simulation, and optimal control of an important industrial process. The results are obtained in close collaboration with engineers and validated by experiments in a pilot hot-rolling mill.

Confirmed speakers

- Dietmar Hömberg, Weierstrass Institute Berlin
- Masahiro Yamamoto, University of Tokyo
- Jens Seidel, Technische Universität Chemnitz.

Models of drift-diffusion for concentrated solutions

Maria Bruna and Barbara Wagner

Keywords: battery electrolytes, interacting particle systems, cross-diffusion system, excluded-volume effect, electrostatic forces, hydrodynamic effects, Poisson-Nernst Planck equation, Fokker-Planck equation

Abstract

Many problems in industry involve particles or ions in solution, and usually most models use an ideal solution approximation (that is, constant diffusivity and/or conductivity). Increasingly, for example in modern battery electrolytes, the concentration of particles is such that the ideal approximation is not sufficient, requiring a concentration-dependent for diffusivity and conductivity. These can be obtained from macroscopic models of the particle system incorporating both short- and long-range interactions. The speakers of this mini symposium will cover a range of problems, both from a mathematical and applications point of view.

We think this session would be appropriate for the material science and semiconductors day.

Speakers

- Giles Richardson or Rahifa Ranom - School of Mathematics, University of Southampton
- Jon Chapman - OCIAM, Mathematical Institute, University of Oxford
- Clemens Guhlke (to be confirmed) - WIAS Berlin, Leibniz Group "Mathematical Models for Lithium-Ion Batteries.
- Marie-Therese Wolfram - Department of Mathematics, University of Vienna
- Luigi Paduano or Roberto Sartorio (to be confirmed) - Chemistry Department, University Federico II in Naples.

Mathematical Modelling of Photovoltaic Devices

Andreas Muench and Barbara Wagner

Keywords: Photovoltaic Devices, Fabrication and Operation and Optical Properties, Mathematical Modelling, Analysis, Computer simulations, Optimisation

Abstract

The development of photovoltaic technologies has been the focus of intensive research in an effort to increase the efficiency and stability of these devices while at the same time bringing down the production price. Much of these advances have relied on improving existing and new PV concepts via extensive experimentation. The full potential of these technologies however can be exploited by a quantitative understanding and optimisation of the underlying physical processes via mathematical modelling, analysis and computer simulations. This workshop will focus on aspects relevant to fabrication, operation and optical properties of novel concepts for photovoltaic devices.

Proposed speakers

- Viktor Burlakov (University of Oxford)
- Giles Richardson (Univ. Southampton)
- Franck Schmidt/Daniel Lockau (ZIB, Berlin) (to be confirmed)
- Matthey Hennessy (University of Oxford)
- Thomas Koprucki (Weierstrass Institute) (to be confirmed)
- Maciek Korzec (Technical University Berlin)

Bayesian and approximative sampling methods for Uncertainty Quantification

Alexander Bibov, Vladimir Shemyakin, Heikki Haario and Marko Laine

Keywords: Data Assimilation, parameter estimation, state estimation, chaotic systems, filtering

Abstract

The aim of Uncertainty Quantification is to estimate the reliability of model simulations. In addition to the statistical uncertainties due to noisy measurement data, one wants to estimate the impact of model bias and numerical approximations necessary due to high CPU demands or high model state dimensions.

The motive for the methods presented in this mini symposium comes from wheather and climate models. We present methods that enable MCMC sampling for high-CPU systems, as well as approximative filtering methods that enable state estimation of very high-dimensional models. The approaches are applied to parameter estimation of chaotic systems. On the other hand, a no-cost parameter estimation approach is discussed, that is based on monitoring of operational weather predictions. The results are compared to those we obtain by differential evolution algorithms.

Confirmed speakers

- Alexander Bibov, LUT, Finland
- Vladimir Shemyakin, LUT, Finland
- Heikki Haario, LUT, Finland
- Marko Laine, Finnish Meteorological Institute, Finland

Mini-Symposium on Nature's natural order: from individual to collective behaviour and self-organization

H Gadelha and PK Maini

Affiliation and Contact Information of the Organizer(s)

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Short description

Ordered randomness is ubiquitous in nature. Every single biological system, from molecular motor dynamics in intracellular processes, multicellular organisms to human social behaviour, from micro- to macro-scale, is susceptible to arbitrary events, which did not have to happen in a certain way, but which did, and completely defined the final system. Interestingly, despite the inherent complexity of many interacting individual agents, order and structure may arise naturally, producing robust global behaviours with emergent properties that qualitatively differ from those of its individual units. In this mini-symposium, we will explore how mathematical modelling can be utilized to predict and interpret the different facets of self-organization and collective behaviour in biology, establishing what is known and identifying further challenges. The proposed mini-symposium will additionally highlight that this is a fertile and challenging area of inter-disciplinary research for applied mathematicians, while demonstrating the importance of future observational and theoretical studies in understanding the underlying mechanisms of self-organization and collective behaviour.

Motivation/Relevance to ECMI

Within a holistic view, we aim to explore how mathematics is revolutionizing our knowledge in self-organization and collective behaviour in biology,

from artificial systems and animal behaviour at the macro-scale, to molecular motor dynamics and microorganism swarming at the micro-scale. In particular, we investigate how individual and simple agents cooperate to achieve complex tasks and organization, while incorporating the relationship between local and global behaviour. This will further highlight the need to dissolve the boundaries between different areas of knowledge and expertise, and as the natural philosophers, contemplate each phenomenon in its entirety. Thus demonstrating how mathematics is intrinsic to biology.

Confirmed speakers

Dr H Gadelha.

Other proposed speakers

- Dr Radek Erban, Mathematical Institute, University of Oxford, UK
- Dr Ulrich Dobramysl, Mathematical Institute, University of Oxford, UK
- Dr Marco Polin, Physics Department, Warwick University, UK
- Dr Ottavio Croze, Univeristy of Cambridge, UK
- Prof Jean-Franois Joanny, Institut Curie, France
- Prof. Jacques Prost, Institut Curie, France
- Prof Jaume Casadelmunt, Universitat de Barcelona, Spain
- David Oriola, Universitat de Barcelona, Spain
- Hugo Wioland, DAMTP, Univeristy of Cambridge, UK
- Francis G. Woodhouse, DAMTP, University of Cambridge, UK

Model Based Optimization of Industrial Processes

Stefan Körkel and Alexander Badinski

Keywords: Mathematical modeling, Optimization, Industrial processes

Motivation

BASF and IWR Heidelberg have a long tradition of cooperation in modeling, simulation and optimization of industrial processes. This minisymposium discusses recent methodological developments, path-breaking application cases and future challenges.

Confirmed speakers

- R. Kircheis et al. Validation of Enhanced Oil Recovery Models
- M. Kudruss et al. Optimization of Robot Motions
- S. Koerkel et al. A Virtual Laboratory for Nonlinear Processes
- A. Badinski et al. Optimization of Industrial Biotechnological Processes

Other Proposed Speakers: e.g.
Contribution from the Kostina Group, Marburg
Contribution from the Schulz Group, Trier
Contribution from the Diehl Group, Freiburg
Contribution from the Wozny Group, Berlin

Industrial Participation

This MS is co-organized by A. Badinski, BASF SE, Ludwigshafen. It discusses projects from industrial-academic cooperation.

Network processes and differential equations

Andras Batkai and Peter L. Simon

Keywords:network processes, differential equations, numerical analysis

Organizers

András Bátkai and Peter L Simon, Institute of Mathematics, Eötvös Loránd University, Budapest Hungary. (simonp@cs.elte.hu)

Abstract

The aim of this mini symposium is to present results about modeling network processes by using ODEs and PDEs. The focus is on the relation between the structure of the network and the qualitative behavior of the solutions of the corresponding differential equations.

Proposed speakers

- Istvan Z Kiss: Exact non-linear ODE models of epidemic propagation on networks with special structure
- András Bátkai: PDE approximation of network processes: a semigroup theoretic approach
- James Gleeson: Modelling choice dynamics on networks
- István Faragó: Network processes and their numerical simulation based on PDE's.
- Peter L Simon: Controlling epidemic propagation on a network

Numerical methods for stiff problems in partial differential equations and applications

Sebastiano Boscarino and Giovanni Russo

Keywords: Partial differential Equations, Stiff problems, Time scales.

Organizers

András Bátkai and Peter L Simon, Institute of Mathematics, Eötvös Loránd University, Budapest Hungary. (simonp@cs.elte.hu)

Abstract

The goal of this mini-symposium is to consider some aspect related to the numerical treatment of stiff problems in partial differential equations (PDEs). Stiff problems arise when a system presents very different time scales.

Typically, the behaviour on the fast scale is dissipative, and classical implicit schemes may be very effective. In other problems, the fast scale describes high oscillatory behaviour. In such cases one has to resort to different strategies, such as exponential methods and/or asymptotic analysis. Numerical methods for time dependent PDEs often use the method of lines approach as the basic concept to separate time and space discretization. When a system comes from the discretisation of an evolutionary partial differential equation, interesting stiff problems arise. For example, the stiffness of the problem may be space dependent, and standard discretization based on a method of lines approach may be inefficient, or in many case the stiffness may be expressed by a small parameter.

This mini-symposium brings together a number of researchers who have been working on the development and testing numerical methods for stiff problems for a variety of partial differential equations with applications.

Relevance to Ecmi

Many problems of great interest for industry are characterised by different time scales. Here we mention models in combustion, kinetic models near the fluid dynamic limit, long time behaviour of mechanical systems, just to mention a few examples.

Confirmed Speakers

- Martin Frank, MATHCCES Department of Mathematics, RWTH Aachen University;
- Jingmei Qiu, Department of Mathematics, University of Houston;
- Francis Filbet, Institut Camille Jordan, Université Claude Bernard, University of Lyon;
- Mattia Penati, MOX - Politecnico di Milano.

Recent advances on equilibrium problems with applications to networks

Patrizia Daniele

Keywords: Optimality conditions, Variational formulation, Duality, Projected Dynamical Systems, Supply Chains

The problem of users of a congested transportation network seeking to determine their travel paths of minimal cost from origins to their respective destinations is a classical network equilibrium problem. There is also an economic interpretation where the demand side corresponds to consumers of the network and the supply side is represented by the network itself, with prices corresponding to travel costs. Many other applications of equilibrium problems can be find in the field of industry, finance, engineering, telecommunications,

The aim of the mini-symposium is to present the new advances on equilibrium problems associated to social and economic world.

Confirmed Speakers

- Anna Nagurney, Department of Operations and Information Management, Isenberg School of Management, University of Massachusetts, Amherst
- Monica Gabriela Cojocaru, University of Guelph, Ontario, Canada
- Fuminori Toyasaki, School of Administrative Studies, York University, Toronto, Canada
- Laura Scrimali, Department of Mathematics and Computer Science, University of Catania, Italy
- Fabio Raciti, Department of Mathematics and Computer Science, University of Catania, Italy
- Patrizia Daniele, Department of Mathematics and Computer Science, University of Catania, Italy

Mini-Symposium on Particle methods and their applications

Giuseppe Bilotta
and Alexis Hérault

Affiliation and Contact Information of the Organizer(s)

Giuseppe Billotta, Istituto Nazionale di Geofisica e Vulcanologia, Sezione di Catania, Italy, giuseppe.bilotta@ct.ingv.it

Alexis Hrault, Conservatoire National des Arts et Mtiers, France, alexis.herault@cnam.fr

Short description

Particle methods such as Smoothing Particle Hydrodynamics (SPH) are Lagrangian, meshless numerical method for Computational Fluid Dynamics (CFD) which has recently seen a growing interest in a wide variety of problems, including hydrodynamics, multi-fluid simulations, thermal problems, lava flow simulations, fluid-structure interaction problems, with applications ranging from oceanography to medicine, from engineering to geophysics.

The purpose of the mini-symposium is to present the current state-of-the-art in applied particle methods, both for scientific research and in industrial applications.

Motivation/Relevance to ECMI

Our motivation in proposing the Smoothed Particles Hydrodynamics and its applications mini-symposium at ECMI is to provide an opportunity for researchers and applied mathematicians working on and with particle methods to present their work both to fellow scientists in the same research fields and to a wider audience. We believe that the mini-symposium is of interest for ECMI for two main reasons. Firstly, particle methods are a powerful and flexible tool for computational fluid-dynamics of great relevance for environmental and industrial applications; secondly, the mini-symposium will provide an opportunity for researchers coming from a different background to gain a new perspective on SPH as a tool for numerical simulations. We

aim to attract interest among scientists and engineers that could provide new opportunities on potential applications of particle methods

Confirmed speakers

- Giuseppe Bilotta (INGV, DMI), Alexander Vorobyev, Alexis Hérault (CNAM), Damien Violeau (EDF), Ciro Del Negro (INGV): *SPH for the simulation of a dam-break with floating objects*
- Sudarshan Tiwari, Axel Klar, Steffen Hart (UniKL): *Numerical simulation of wetting phenomena by a meshfree particle method*
- Peep Miidla, Jri Liiv, Aleksei Mashirin and Toomas Tenno: *Simulation of a twisting-ball display cell*
- Eugenio Rustico (BAW), Béla Sokoray-Varga (BAW), Giuseppe Bilotta (INGV, DMI), Alexis Hérault (CNAM), Thomas Brudy-Zippelius (BAW): *Full 3D numerical simulation and validation of a fish pass with GPUSPH*

Affiliations

- INGV, Istituto Nazionale di Geofisica e Vulcanologia, Italy
- DMI, Dipartimento di Matematica e Informatica, Università di Catania, Italy
- CNAM, Conservatoire National des Arts et Métiers, France
- EDF, Électricité de France
- BAW, Bundesanstalt für Wasserbau, Germany
- UniKL, University of Kaiserslautern, Germany

Mini-Symposium on Mathematical Methods in Photoacoustic Tomography and Optical Coherence Tomography

Peter Elbau[48] *and Leonidas Mindrinos*[49]
[50]

Short description

Photoacoustic Tomography (PAT) and Optical Coherence Tomography (OCT) are both non-invasive imaging techniques producing high-resolution images of biological tissues. To model the light propagation within the sample, the radiative transfer equation in PAT and the Maxwell equations in OCT are mainly used. Both inverse problems consist of determining the optical properties of the sample. In general, without any assumptions about the medium, it is not possible to reconstruct all the optical coefficients. New applications consider the combination of PAT and OCT to achieve increased functionality. From a mathematical point of view, this dual model is not yet sufficiently developed. Thus, the scope of this mini-symposium is to bring together researchers from both fields to present recent developments and exchange ideas for future challenges.

Motivation/Relevance to ECMI

PAT and OCT are emerging techniques in biomedical imaging and diagnostics. Cancer detection, ophthalmology and skin abnormalities detection are some applications. Mathematical theory and methods arise from those modern life sciences are relevant to ECMI. New challenges concern not only reconstruction algorithms but also theoretical aspects.

Confirmed speakers

Dr H Gadelha.

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Other proposed speakers

- Peter E. Andersen, Department of Photonics Engineering, Technical University of Denmark, Denmark.
- Simon R. Arridge, Department of Computer Science, Department of Mathematics, University College London (UCL), United Kingdom.
- Zakaria Belhachmi, Mathematics, Information Technology and Applications Laboratory, Mulhouse Cedex, France.
- Maïtine Bergounioux, Department of Mathematics, Université d' Orléans, France.

Mini-Symposium on Advanced Imaging for Industrial Application

Sebastiano Battiato,
Giovanni Gallo,
Filippo Stanco

Affiliation and Contact Information of the Organizers

Università di Catania,
Dipartimento di Matematica e Informatica,
viale A. Doria n. 6,
95125 Catania

Short description

The aim of this mini-symposium is to provide an overview of state of the art methods for imaging applications in different industrial contexts (consumer devices, e-health, digital signage, forensics, Cultural Heritage, etc.) to stimulate the creation of appropriate benchmark dataset to be used as reference for the development of novel algorithms.

Motivation/Relevance to ECMI

The conference ECMI includes as main topic the *imaging* and in our mini-symposium will be original contributions which address a wide range of theoretical and practical issues related to the application of digital image processing techniques to various aspects of industrial contexts.

Confirmed speakers

- Cosimo Distante, Marco Leo - CNR Lecce
- Alessandro Capra STMicroelectronics
- Domenico Tegolo - Universit di Palermo
- E. Ardizzone - Universit di Palermo.

Industrial participation

STMicroelectronics

Mini-Symposium on Optimization and Optimization-based Control Methods for Industrial Applications

Dr. Kathrin Flaßkamp [5152]
and Dr. Timm Faulwasser [5354]

Short description

The increasing need for resource and energy efficiency in industrial applications leads to manifold scientific and technical challenges in the design and operation of industrial systems and processes. Typical examples of such challenges are, for instance, energy-efficient operation close to safetycritical constraints, online determination of optimal operation policies and the need for an optimal tradeoff between conflicting objectives. Mathematical optimization and optimal control methods are key enabling technologies to tackle some of these challenges. They play a crucial role in various fields of applications ranging from aeronautics and aerodynamics, automotive, space mission design, and robotics to biomechanics and process industries.

The aim of this mini-symposium is to provide an overview of current trends of mathematical optimization and optimization-based control methods for industrial applications. Thus, we invite speakers from applied mathematics as well as from control engineering. In particular, a platform for scientific exchange and collaboration of young scientists shall be provided. The list of authors of confirmed talks includes scientists from Germany, Switzerland and Australia. Furthermore, the minisymposium supports the exchange of ideas between industry and academia, providing insight to open problems and state of the art in industry to young researches and show novel solution methods and opportunities to representatives from industry. One of the confirmed talks presents a collaboration with Hella KGaA Hueck & Co., a global automotive supplier. Another confirmed talk on optimal control for autonomous helicopters will even be presented by an employee of the DLR (national aeronautics and space research centre of the Federal Republic of Germany).

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[54]ME C2 392 Station 9 CH-1015 Lausanne Phone: +41 21 69-37341 Mail: timm.faulwasser@epfl.ch

Confirmed speakers

- Sebastian Peitz, Michael Dellnitz, Kathrin Flaβkamp, Christian Horenkamp, (University of Paderborn), Sina Ober-Blöbaum (TU Dresden), Julian Eckstein, Patrick Friedel, Ulrich Köhler, Sebastian Tiemeyer (Hella KGaA Hueck & Co.): *Multiobjective optimal control for an electric vehicle*

- Johann Dauer, Sven Lorenz (DLR Braunschweig), Timm Faulwasser (Ecole Polytechnique Federale de Lausanne): *Computational aspects of optimization-based path following of an unmanned helicopter*

- Philipp Braun, Lars Grüne (University of Bayreuth), Karl Worthmann (TU Ilmenau), Christopher Kellett, Steven Weller (University of Newcastle): *Distributed Model Predictive Control for a Smart Grid Application*

- Jürgen Pannek (University of Bremen): *Optimization in Container Temperature Control* (participation confirmed, title and list of coauthors are tentative)

- Sabrina Fiege, Andrea Walther (University of Paderborn), Andreas Griewank (HU Berlin): *A bundle method for piecewise linear problems.*

Modeling and Optimization of Interacting Particle Systems

Rene Pinnau, Claudia Totzeck, Jochen Kall and Stephan Martin

Keywords: modeling, optimization, interacting particle systems, biology, semiconductors

The aim of this mini symposium is to present recent advances in the modeling, simulation and optimization of interacting classical and quantum particle systems with applications in biology and semiconductor device modeling.

Speakers

- Rene Pinnau, TU Kaiserslautern, Germany
- Claudia Totzeck, TU Kaiserslautern, Germany
- Jochen Kall, TU Kaiserslautern, Germany
- Stephan Martin, Imperial College, UK

Mini-Symposium on Multiphysics simulations with industrial applications

Stefano Micheletti and Simona Perotto[55]

Short description

Many problems in engineering and applied sciences are characterized by a coupling among several physical fields. This involves a strong interaction of different disciplines. Remarkable instances are provided by fluid-structure interaction problems, structural-pore pressure coupling or Micro-Electro-Mechanical Systems (MEMS). The mathematical modeling and numerical simulation of multiphysics problems is still an ambitious challenge for the scientific computing.

Goal of this mini-symposium is to provide some examples of multiphysics modeling with a particular emphasis on industrial applications.

Motivation/Relevance to ECMI

This mini-symposium exactly fits ECMI's topics of interest since multiphysics processes are thoroughly transverse to mathematics for industry.

Confirmed speakers

- Simone Pezzuto, Simula Research Laboratory, Norway
- Suzanne M. Shontz, Mississippi State University, USA
- Marianna Signorini, MOX, Politecnico di Milano, Italy
- Timo van Opstal, SINTEF ICT and Norwegian University of Science and Technology, Norway

Speakers to be confirmed

- J. Peir, Imperial College, UK

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- P.E. Farrell, University of Oxford, UK

Two other speakers will be contacted shortly.

Simulation Issues for Nanoelectronic Coupled Problems

Caren Tischendorf

Keywords: nanoelectronics, coupled problems, time-domain simulation, model order reduction, multirate methods, partial differential algebraic equations

This minisymposium addresses simulation issues for the design development in nanoelectronics. In order to meet the challenge of large-size simulation problems involving EM-circuit-heat couplings the following mathematical topics shall be covered: co-simulation and coupled monolithic simulation methods for partial differential algebraic equations, multirate envelope methods, reduced basis methods for stochastic partial differential equations and parameterized model order reduction approaches.

Motivation/Relevance to ECMI and Industrial Participation

This minisymposium is devoted to a broad dissemination of recent advances of the European collaborative research project nanoCOPS in which eight academic partners, two large-scale semiconductor companies and two SMEs develop, extend and validate design tools for nanoelectronic IC and EM simulation.

Speakers

- Jan ter Maten (University of Wuppertal, Germany)
- Lihong Feng / Peter Benner (Max Planck Institute for Dynamics of Complex Technical Systems, Germany)
- Sebastian Schöps (University of Darmstadt, Germany)
- Caren Tischendorf (Humboldt University of Berlin, Germany)

Other proposed speakers: Wil Schilders (Eindhoven University of Technology, The Netherlands), Rick Jansen (NXP semiconductors, The Netherlands), Hans-Georg Brachtendorf (University of Applied Sciences Upper Austria, Austria)

Multiphsyics simulation in electrical engineering

Michael Günther, Wuppertal

Keywords: multiphysics simulation, electrical engineering, industrial mathematics

Abstract

The research consortium *Model-reduction-based simulation of coupled PDAE problems* (KoSMOS) funded by the German Federal Ministry of Education and Research (BMBF) is concerned with the modelling, analysis and simulation of complex multi-disciplinary problems, which usually lead to PDAE systems. The large dimension of the space-discretized equations as well as the heterogenity of system components demands for the development of new efficient algorithms, which combine model order reduction, modular time integration and multirate approaches. The consortium thus aims at analysing model-order-reduction-based simulation methodologies for coupled PDAE and multiscale systems, which allow both for a fast simulation based on the modular structure and higher accuracy and robustness. The consortium consists of three university partners (University of Augsburg, Humboldt-University of Berlin and University of Wuppertal) and three companies (CST, ITI and Kostal).

Speakers

- Johanna Kerler (University of Augsburg): Nonlinear model reduction for simulation of coupled systems
- Lennart Jansen (Humboldt University Berlin): Numerical simulation of PDAEs for water transportation networks
- Christof Hachtel (University of Wuppertal): Multirate schemes and model order reduction
- NN (a talk from one of the industry partners - will be fixed soon)

Current challenges in Computaional Finance

Claudio Albanese

Keywords: Computational finance, Finite difference, Portfolio simulation

Abstract

In the aftermath of the crisis, the computational challenges in Finance have been shifting from exotic derivative pricing to the simulation of large complex portfolios of simpler instruments. This symposium focuses on emerging problems and challenges in this area.

Speakers

- Sebastian Del Bano Rollin, Department of Mathematics,
- University College London
- Giacomo Pietronero Global Valuation, London
- Claudio Albanese, Global Valuation, London
- Damiano Rossello, University of Catania

Mini-Symposium on Mathematics in Nanotechnology

T. G. Myers[1], *Luis Bonilla*[2]

Affiliation and Contact Information of the Organizer(s)

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Motivation/Relevance to ECMI

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

Confirmed speakers

- Mariano Alvaro (UC3M, Madrid)
- Luis Bonilla (UC3M, Madrid)
- Ana Carpio (Complutense, Madrid)
- Fran Font (CRM, Barcelona)

- Tim Myers (CRM, Barcelona)
- Vincent Cregan (CRM, Barcelona)

Efficient Numerical Simulation of the Wilson Flow in Lattice QCD

Michèle Wandelt and Michael Günther [56]

Abstract

Lattice Quantum Chrome Dynamics (Lattice QCD) is a gauge theory formulated on a highly dimensional grid or lattice of points in space and time. It aims at determining observables such as the mass of elementary particles as accurate as possible, with computational costs as low as possible at the same time. Thus high performance computing tools are inevitable, as well as the construction of HPSC hardware tailored to the needs of Lattice QCD. In the Hybrid Monte Carlo (HMC) approach, Monte Carlo simulations involving a molecular dynamics step in its core are performed, which yield physical values provided with their statistical errors.

In this talk we concentrate on theWilson Flow, a system of differential equations defined on the Lie group SU(3). The Wilson Flow can be used, e.g., to determine the physical lattice spacing which influences the result of the HMC simulations.We focus on tailored Runge-Kutta Lie group integration methods with step size prediction. The numerical results confirm that our strategy reduces the statistical errors of the simulation.

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Ab-initio based Kinetic and Transport Models

Antonino La Magna

Author Keywords: Multiscale modelling, Ab-initio techniques, Density Functional Theory, Molecular Dynamics.

Transport simulation methods must reproduce the microscopic evolution of real materials in order to be properly applied to problems of industrial interest. This requirement is the sufficient condition to get reliable predictions from the kinetic models without any "ad hoc" fitting procedure. Anyway, the mechanisms ruling the kinetics at the atomic scale is barely accessible by any experimental technique. In this respect, accurate calculations in the framework of the Density Functional Theory (DFT) or Molecular Dynamics (MD) can significantly aid the unbiased development and the correlated parameter calibration of transport models; whist the experiments can be used only for the model validation by means of the comparison between the modelling prediction on macroscopic observables and the experimental data. Indeed, "ab-initio" approaches can calculate in small system of the nanometer scale the atomic properties of a given material or material system (e.g. an interface) specifying the atomic constituents of the system without, in principle, any relevant approximations. As a consequence the fundament of the predictivity potential of the kinetic model derives from the proper matching of the DFT/MD calculated "information" (e.g. material parameters, atomic configuration, migration/diffution paths, energetics, electronic structure, etc) in the simulation scheme. The latter approach can efficiently simulate large systems for long times, i.e. at the scale of industrial processes and devices. In this mini-symposium important examples of this coupled numerical technique will be discussed by the speakers.

Relevance to ECMI

Multiscale modelling is a key element of the modern mathematical and numerical modelling. The industrial application needs the reduction of the general formalisms to specific problematic. Ab-initio techniques coupled to kinetic and transport models are the appropriate answer to this requirement on the basis of a pure theoretical/computational approach.

A Hydrodynamical model for charge and heat transport in graphene

Giovanni Mascali and Vittorio Romano.

Author Keywords:Charge Transport, Heat Transport, Graphene.

Abstract

Graphene is a two dimensional material which has very good mechanical properties and is an excellent heat and electricity conductor. In very high quality graphene very few defects are present, which makes the contribution of phonons to room temperature resistivity very important and motivates the formulation of comprehensive transport models taking into account electrons in the conduction and valence bands, as well as phonons. In this paper we present a model for a suspended sheet of graphene.

Deterministic simulation of a DG-MOSFET through a parallel solver

Francesco Vecil

Author Keywords:DG-MOSFET, Deterministic simulation, Boltzmann-Schrodinger-Poisson system.

Abstract

We present a deterministic solver for a DG-MOSFET described by a Boltzmann-Schrodinger-Poisson system. The model is hybrid in the sense that the electrons are described as waves along the confined dimension and as particles along the longitudinal one.

In this work we focus on obtaining physically accurate results by using realistic Si conduction band and seven electron-phonon scattering phenomena. The code being accurate but computationally costly, it has been parallelized following a domain-decomposition approach.

The results have been compared to those given by a Monte-Carlo solver, over which the deterministic strategy has the advantages of being noise-free and of properly describing almost-empty zones.

Approximate Uncertainty Quantification Using Vague Knowledge

S. Subbey, B. Planque, U. Lindstrøm, A. Frank[57]

Abstract

We explore the stochastic dynamics of a simple foodweb system using a network model which mimics interacting species in a biosystem. It is shown that the system can be described by a set of ordinary differential equations whose dynamics is governed by a finite set of unknown and highly uncertain parameters, $\mathbf{p} \in \mathbb{R}^k$, such that

$$B\mathbf{p} \leq \mathbf{b} \tag{1}$$

where $B \in \mathbb{R}^{s\times k}$ and $\mathbf{b} \in \mathbb{R}^s$ are known. Equation (1) restricts the solution space of $\mathbf{p}$ to a bounded convex polytope, C.

We present numerical experiments to demonstrate that the stochasticity and uncertainty characterizing the system can be captured by an approximate sampling of the parameter space using a prescribed probability density function, f , over C. The example illustrates a parsimonious approach to modeling and uncertainty quantification using vague knowledge of complex biosystems.

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Tracking Uncertainty Propagation in a Fisheries Population Dynamics Model

S. Subbey, H. Skaug, L. Frimannslund[58]

Abstract

This paper presents a framework for combining uncertain data from multiple sources in an age-structured statistical population model to assess the population size of a fish stock. The framework accounts for data and model parameter uncertainties, and allows us to track how these uncertainties propagate through the modeling process to affect model predictions and other derived parameters.

The model parameters are estimated using Automatic Differentiation (AD) [3], implemented on the ADMB [1] platform, and the uncertainty quantification is based on a Markov Chain Monte Carlo (MCMC) approach [2].

Using numerical experiments, we demonstrates that the combination of AD and MCMC aproach provides a robust framework for parameter estimation and uncertainty quatification.

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Main Track

An alternative stochastic volatility model

Youssef El-Khatib [59] Abdulnasser Hatemi-J [60]

Abstract

Stochastic volatility modelling is of fundamental importance in financial risk management. Among the most popular existing models in the literature are the Heston and the CEV stochastic models. Each of these models has some advantages that the other one lacks. For example, the CEV model and the Heston model have different relative properties concerning the leverage as well as the smile effects. In this work we suggest a new stochastic volatility model that is based on the CEV and the Heston models combined. This new model is expected to perform better than any of the two previously mentioned models in terms of dealing with both the leverage and the smile effects. We deal with the pricing and hedging problems for European options. We first find the set of equivalent martingale measures (E.M.M.). The market is found to be incomplete within this framework since there are infinitely many of E.M.M.We then find the targeted E.M.M. by minimizing the entropy. Using Ito calculus and risk-neutral method enable us to find the partial differential equation (P.D.E.) corresponding to the option price. Moreover, we use Clark-Ocone formula to obtain a hedging strategy that minimizes the distance between the payoff and the value of the hedged portfolio at the maturity. This hedging strategy is the most effcient one among all the available strategies.

Keywords: Asset Pricing and Hedging, Options, Stochastic Volatility

[59] Mathematics Subject Classification (2010): 91B25, 91G20, 60H07.
[60] JEL Classification: C02, G01, G11, G12, G13

Model, CEV Model, Heston Model.

Global existence of weak solutions to an angiogenesis model

N. Aïssa , USTHB, Laboratoire AMNEDP [61]

Abstract

Abstract We prove global existence of a weak solution to the angiogenesis model proposed by A. Tosin, D. Ambrosi, L. Preziosi in Bull. Math. Biol. (2006) 7;1819-1836: The model consists of compressible Navier-Stokes equations coupled with a reaction-diffusion equation describing the concentration of a chemical solution responsible of endothelial cells migration and blood vessels formation.

Proofs are based on the control the entropy associated to the hyperbolic equation of conservation mass and the adaptation of the results of P.L. Lions dealing with compressible fluids which are inevitable for all models dealing with compressible Navier-Stokes equations.

We use the vanishing artificial viscosity method to prove existence of solutions, the main difficulty for passing to the limit is the lack of compactness due to hyperbolic equation which usually induces resonance phenomenon. This is overcome by using the concept of the compactness of effective viscous pressure combined with suitable renormalized solutions to the hyperbolic equation of mass conservation.

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Deformation of liquid drops and thin-films under the influence of an electric field

Nigel Mottram

Author Keywords: Dielectriphoresis, Microfluidics, Droplet, Fluid dynamics

Abstract

The ability to control the shape of droplets and thin films of liquid, via an externally applied electric field, has been exploited for technological applications including surface tension measurements, ink-jet printing, optical displays, and optimising the properties of polymer microlenses. Working with experimental collaborators at Nottingham Trent University we consider a system where a sessile droplet or film is placed on one substrate of a parallel plate capacitor. Experimentally we see that the liquid-air interface within the capacitor is distorted at low electric field strengths and, in some cases, an instability leads to the liquid bridging between the two capacitor plates.

Our work aims to describe the static and dynamic interface distortions as a function of key experimental parameters (droplet size, capacitor plate separation, electric field magnitude and contact angle). We derive straightforward analytical scaling relationships for static distortions, and a system of partial differential equations with the inclusion of fluid flow to describe the dynamics of distortions. Our approach avoids the requirement for detailed numerical methods in certain limiting cases, in particular for thin films or for droplets with contact angles of either almost 90 degrees or close to 0 degrees.

We investigate the limits of validity of these equations and compare with real experimental geometries with a range of liquids using fast imaging and optical interferometry.

Numerical simulation of heat transfer in underground electrical cables

R. Čiegis[62] and G. Jankevičiūtė [63] and A. Bugajev and N. Tumanov

Abstract

The aim of this project is to develop a virtual modelling tool which can be used to construct optimal design of power transmission lines and cables. They should meet the latest power transmission network technical and economical requirements. The mathematical model is based on a general heat conduction equation

$$\rho_c(X,T)\frac{\partial T}{\partial t} = \sum_{\ell=1}^{2}\frac{\partial J_\ell}{\partial x_\ell} + q(1+\alpha(T-T^*))I^2, \quad X \in D, \tag{2}$$

$$J_\ell = \lambda(X,T)\frac{\partial T}{\partial x_\ell} + \nu_\ell(X,T)T, \quad \ell = 1,2,$$

where T is temperature in in the Kelvin scale, $\lambda > 0$ is the heat conductivity coefficient, $\rho > 0$ is the mass density, $c > 0$ is the specific heat capacity, I represents an electric current. We take into account a linear dependence of the resistance on temperature, T^* is the reference temperature. Functions ν_ℓ define the convective transport of the heat in air regions, they are obtained by solving a coupled thermoconvection problem including the heat

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conduction problem (2) and a standard Navier-Stokes model of the flow in air. The changes of material coefficients in soil due to influence of heating are taken by solving a simplified mass balance equation for flows in porous media. The FVM is used to solve the obtained system of differential equations. Discretization of the domain is done by applying *aCute* mesh generator, which is a modification of the well-knowm Triangle mesh generator. The discrete schemes are implemented by using the OpenFOAM tool. Parallel versions of basic algorithms are also investigated. Results of computational experiments of simulation of real industrial underground cables are presented.

The stochastic Poisson and Poisson-Boltzmann equations applied to quantifying noise and fluctuations in nanoscale sensors

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Abstract

Nanowire bio- and gas sensors showing impressive sensitivity have been fabricated in recent years. At the same time, however, quantitative understanding of noise and fluctuations in these devices is still missing, although it is important for determining detection limits.

Hence we use stochastic partial differential equations (SPDEs) in order to quantify uncertainties, noise, and fluctuations and to go beyond the calculation of averages. The main model equations are the (linear) Poisson equation and the (nonlinear) Poisson-Boltzmann equation. We report deterministic and stochastic homogenization results, and we discuss our numerical algorithms for these types of problems. Finally, we present simulation results going from stochastic processes as the input to noise and fluctuations in the current through the sensors as the output.

(Support by the FWF (Austrian Science Fund) START project no. Y660 PDE *Models for Nanotechnology* is acknowledged.)

An inverse problem for a generalized transport equation in polar coordinates

İsmet Gölgeleyen

Author Keywords: Inverse problem, generalized transport equation, polar coordinates.

Abstract

We consider the inverse problem of the determination of the right hand side of a generalized transport equation from boundary measurements. The problem is originally related to an integral geometry problem along a family of curves whose curvature is given by the Christoffel symbols. The solvability of the problem is proven in polar coordinates.

αAMG based on Weighted Matching for Systems of Elliptic PDEs arising from Displacement and Mixed Methods

Pasqua DAmbra and Panayot S. Vassilevski [64]

Abstract

Adaptive Algebraic Multigrid Methods (αAMG) are introduced to improve robustness and efficiency of classical algebraic multigrid methods in dealing with problems where no a-priori knowledge or assumption of the near-null components of underlined matrix are available. Recently, in [1], we proposed an αAMG based on a bootstrap strategy aimed to obtain a composite solver with a desired convergence rate. Each new multigrid component relies on a current (general) smooth vector and exploits pairwise aggregation based on weighted matching in a graph to build efficient coarse hierarchy and respective interpolation operators. More specifically, we apply weighted matching

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algorithms to the adjacency graph of the system matrix, which was successfully exploited for designing reordering algorithms to enhance diagonal dominance in sparse direct methods. The latter, combined with the concept of compatible relaxation, made it possible to define an automatic, generalpurpose coarsening process, which we refer to as *the compatible weighted matching*. It does not require any parameters as in the classical AMG characterization of strength of connection between the variables. In this work, we present results that extend the application of our method to different systems of elliptic PDEs arising from the finite element method. In particular, we consider systems arising from displacement methods in linear elasticity problems and saddle point systems that appear in the application of the mixed method to Darcy problems.

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Modelling the ripening of cheddar cheese

Winston Sweatman

Author Keywords: mathematics in industry study group, modelling cheese, dairy produce

Abstract

Cheese undergoes a number of ripening processes as it matures. These processes were mathematically modelled in a project brought to the 2013 mathematics-in-industry study group at Queensland University of Technology, Brisbane (MISG 2013). Such models could be useful for predicting the quality of cheese using initial measurements. This talk will consider the main results and ongoing investigation.

This project had a particular focus on cheddar cheese. The main ripening processes are modelled with chemical reactions governed by differential equations. These contain a number of unknown parameter values which are fitted using experimental data presented in the literature. Numerical integration is used for simulating the system represented by the equations. In general, the results of numerical fitting are in good agreement with experimental data.

Fiber suspension flows: simulations and existence results

Uldis Strautins [65]

Abstract

The research field of fiber suspension flows constitutes a rich example of interplay between abstract theory and practical application. Understanding the process is cruical for certain fields in industry, leading to a rich variety of models which require special simulation techniques, but also analysis of the underlying mathematical properties. There have been several efforts to estabilish the well posedness of certain models and hence justify the existence of the solution as a valid target for numerical methods. The well posedness has been estabilished for the case of linear equations for the fiber orientation variables [2]. A procedure to show well posedness for nonlinear equations locally in time for sufficiently small data has been demonstrated [1]. This can be extended to a wide class of related models [3], however, not for the classical Folgar-Tucker model containing the shear rate $\dot{\gamma}$, which is not differentiable at the origin. In this talk we demonstrate that the local existence result can be extended to a global in time existence result if we can bound the L^∞ norm of fiber orientation variable, which is the case for the momenta of distribution functions.

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Mathematical formulation of Bioventing Optimal Design Strategies

Filippo Notarnicola[66]

Abstract

Bioventing is a technology used to abate the presence of pollutants in the subsoil.

Microorganisms biodegrade the pollutant but the biochemical reaction requires oxygen and so an airflow is induced in the subsoil by means of injection and/or extraction wells.

Costs, final result and decontamination time are reliant on contaminant type, soil permeability and several other factors, but oxygen subsoil concentration plays a very important role. For this reason a rational choice of well location and flow rate is required.

The mathematical definition of the optimal design problem will be set-up starting from a simplified mathematical model describing the bioventing system.

A formal definition of decontaminated subsoil will be given and the set of system control variables will be identified. Several optimimization strategies such as cost minimization, removal rate maximization and time optimization will be mathematically described.

Keywords: subsoil pollutant removal, bioventing, optimal design, porous media, subsoil fluid dynamics, mathematical modelling.

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A nonlinear CVFE scheme for a degenerate parabolic reaction-diffusion system modeling the volume-filling effect for a chemotaxis model

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Keywords: Reaction-Diffusion System. Volume-Filling Chemotaxis. Control Volume Finite Element Method. Discrete Maximum Principle.

Degenerate parabolic reaction-diffusion systems appear frequently in the modeling of many real life applications. One of the most popular applications is the modeling of chemotaxis.

Chemotaxis is the feature movement of a cell along a chemical concentration gradients. The Keller-Segel model [1] provides a base for the theoretical and mathematical modeling of chemotaxis, it is governed by a parabolic equation modeling the interaction between the cell density and the chemoattractant concentration. Moreover, this equation is coupled by another parabolic equation modeling the diffusivity of the chemeoattractant.

In terms of numerical analysis, a finite volume scheme [2] is developed for the degenerate Keller-Segel model over a homogeneous domain, where the diffusion tensors are considered to be proportional to the identity matrix. However, the finite volume scheme does not permit to handle anisotropic diffusion tensors on general meshes, even of the orthogonality condition is satisfied.

Recently, the convergence analysis of a control volume finite element scheme [3] for degenerate anisotropic Keller-Segel model has been studied. In this scheme, degrees of freedom are assigned to vertices of a primal triangular mesh, as in finite element methods. The diffusion term which involves an anisotropic and heterogeneous tensor is discretized on a dual barycentric mesh (known as Donald mesh) using the diffusion fluxes provided by the conforming finite element reconstruction on the primary mesh. The other terms are discretized using an upwind finite volume scheme on the dual mesh. However, the scheme ensures the validity of the discrete maximum principle under the assumption of the nonnegativity of the transmissibility coefficients.

Our motivation is a new nonlinear control volume finite element scheme for degenerate anisotropic Keller-Segel model. The idea of this scheme is based on the use of each of the Godunov scheme and a nonclassical upwind finite volume scheme to ensure the discrete maximum principle without any restriction on the transmissibility coefficients.

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Numerical study of forced MHD convection flow and temperature around periodically placed cylinders

Harijs Kalis and Maksims Marinaki[67]

Abstract

In many physical experiments and technological applications it is important to mix and heat an electroconductive liquid. Liquid metals are considered to be the most promising coolants for high temperature applications, like nuclear fusion reactors, because of the inherent high thermal diffusivity, thermal conductivity and hence, excellent heat transfer characteristics. In the developed mathematical models, vortex-type structures appear in liquid and air flows, as well as in problems related to energy conversion in new technological devices. MHD convection flow of a viscous incompressible fluid around cylinder with combined effects of heat and mass transfer is an important problem, prevalent in many engineering applications. These types of problems find application in nuclear reactor cooling system and energy transport system. Heat exchanger systems are employed in numerous industries. Steam generation in boiler, air cooling within the coil of an con-

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ditioner and automotive radiators represent just some of the conventional applications of this mechanical system. For the in-line arrangements of tube banks (cylinders), fluid at prescribed mass flow rate of velocity U and an inlet ambient temperature T_0, much lower than the wall temperature T_w, enters the cylinders from the left and exits at the right. By taking the advantage of special geometrical features, such as the inherent repetitive nature of the flow behaviour, the computational fluid domain allows the possible exploitation of symmetric and periodic boundary conditions in speeding up the computations and in turn, enhancing the computational accuracy of the simplified geometries.

Acknowledgements This work was partially supported by the grant 623/2014 of the Latvian Council of Science.

Numerical solution of axisymmetric eddy current problems with hysteresis

Alfredo Bermúdez, Dolores Gómez[68], Rodolfo Rodriguez[69], Pablo Venegas[70]

Abstract

This work deals with the mathematical analysis and the computation of transient electromagnetic fields in nonlinear magnetic media with hysteresis [3]. The problem arises in the framework of a research contract with the Spanish company ORONA, which was devoted to the study of electrical machines. The results obtained complement those in [1, 2], where the mathematical and numerical analysis of a 2D nonlinear axisymmetric eddy current model was performed under fairly general assumptions on the **H-B** curve but without considering hysteresis effects. In our case, the constitutive relation between **H** and **B** is given by a hysteresis operator, i.e., the values of the magnetic induction depend not only on the present values of the magnetic field but also on its past history. We assume axisymmetry of the fields and then we consider two kinds of boundary conditions. Firstly the magnetic field is given on the boundary (Dirichlet boundary

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condition). Secondly, the magnetic flux through a meridional plane is given, leading to a non-standard boundary-value problem. For both problems, an existence result is achieved under suitable assumptions. For the numerical solution, we consider the Preisach model as hysteresis operator, a finite element discretization by piecewise linear functions, and the backward Euler time-discretization.

We report a numerical test which allows us to assess the order of convergence of the proposed numerical method. Finally, we validate the numerical scheme with experimental results.With this aim, we consider an industrial application: the numerical computation of eddy current losses in laminated media as those used in transformers or electric machines.

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Perturbation-analysis for pipe-networks

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We are interested in partial differential algebraic equations (PDAEs) describing flow networks. These PDAEs consist of hyperbolic PDEs of the type

$$p_t + Aq_x = 0$$
$$q_t + Bp_x + H + G(q) = 0$$

which are coupled with algebraic boundary conditions of the type

$$C_1 q(x_R, t) + D_1 q(x_L, t) = q_{set}(t)$$
$$C_2 p(x_R, t) + D_2 p(x_L, t) = p_{set}(t)$$

We use an abstract setting of the form

$$\mathcal{A}^*[\mathcal{D}u(t)]' + \mathcal{B}(u(t), t) = 0$$

with $\mathcal{D}, \mathcal{A} : V \to Z, \mathcal{B} : V \to V^*, t \in \mathcal{I} \subset \mathbb{R}, V \subset Z \subset V^*$ for discussing a perturbation analysis for such PDAEs. We will briefly show that, depending on the chosen spatial discretization, the resulting DAE may have a different perturbation behavior if we consider perturbations in the PDE as well as in the boundary conditions. In particular, the DAE can be of higher index, even though the PDAE is well-posed.

Additionally, we demonstrate that the influence of higher order perturbations diminishes, the finer we chose the discretization. This motivates our approach of regarding the PDAE perturbation index as the limit of the DAE perturbation index under certain assumptions.

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On the problem of reconstruction of a Riemannian metric from the Hodograph

Fikret Golgeleyen

Author Keywords: Riemannian metric, hodograph, integral geometry problem.

We consider the problem of determining a Riemannian metric from the distances between the boundary points of a domain. This problem is related to the problem of determining the sound speed or index of refraction of a medium by measuring the travel times of waves going through the medium. We prove the uniqueness of the solution of the problem for sufficiently wide class of metrics. This is a joint work with Prof. Masahiro Yamamoto and originates from ideas by the late Professor Arif Amirov.

A boundary element method for pricing barriers options

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Keywords: Boundary Element Method (BEM), Barriers Option, Heston model.

The study of phenomena modeled by boundary value problems for partial differential equations is wide in Physics and Engineering but also in Finance and Economics in general.

From 1970s, with the introduction of the electronic computers, Boundary Element Method (BEM) has been largely used and improved in Physics and Engineering and in particular, more recently, its application has been refined for time-dependent problems that involve more difficult theoretical analysis. Despite this, only the very recent contribute by Ballestra ([1]) is available in literature about its application to Quantitative Finance.

BEM is a method for partial differential equations in which a reduction in mesh dimension from a domain-type to a boundary-type is accomplished.

The advantages of BEM, when compared to domain methods, such as Finite Element Methods (FEM) or Finite Difference Methods (FDM), are well known: only the boundary of the domain needs to be discretized, particularly, exterior problems with unbounded domains but bounded boundaries are handled as easily as interior problems. Therefore, this feature makes this method pretty interesting when considering options with single/double barriers: the solution in the domain is approximated with a rather high convergence rate and can be evaluated at particular points of the domain and not necessarily everywhere on a defined grid; infinity conditions are implicitly satisfied. Note that, for plain vanilla options, BEM reduces to the traditional Greens function approach, i.e. the computation of the option price as discounted expectation of the final payoff under suitable probability measure.

One of the main difficulties that could arise applying this method, concerns the necessary explicit knowledge of a fundamental solution for the differential equation that is generally available only for linear partial differential equations with constant or some specific variable coefficients. The

fundamental solution is available in Black-Scholes case but, when considering more complicated models with stochastic volatility (such as Heston model [4]) and jumps (as in Bates model [2]), only the Fourier transform of the fundamental solution is known, so a good strategy has to be carried out to overcome this complication. For Black-Scholes equation, BEM is really efficient and accurate as already deeply investigated in [1] and [3], where the authors have tested the method for different types of barrier options. Here, we will show that this method maintains these qualities also when we dont rely on the analytical expression for the fundamental solution.

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High-order compact schemes for Black-Scholes basket options

Christof Heuer and Bertram Düring

Author Keywords:High-order compact finite difference method, Partial differential equation, Mixed derivatives.

Abstract

We present a new high-order compact scheme for the multi- dimensional Black-Scholes model with application to European Put options on a basket of two underlying assets. The scheme is second-order accurate in time and fourth-order accurate in space. Numerical examples conrm that a standard second-order nite dierence scheme is signicantly outperformed.

Negative Selection - a New Performance Measure for Automated Order Execution

Natasa Krejic, Miles Kumaresan and Sanja Loncar

Author Keywords: automated trading, performance measure, market impact.

Automated Order Execution is the dominant way of executing trade orders for the last couple of years at major stock markets. The most popular performance measures are VWAP (Volume Weighted Average Price) and Expected Shortfall. Both measures are widely used in practice and represent the standard in financial industry. A number of algorithms is developed in order to minimize the slippage to VWAP but VWAP slippage does not always capture the impact of one's own trading activity.

Negative Selection as a performance measure aims at providing an alternative way of measuring the performance of execution algorithm taking a posteriori view of the market conditions and thus resolving some of the drawback present with VWAp and ES. The posteriori approach allow us to determine what would be the optimal order placement if we knew the complete market information during the trading window. Thus we define the performance measure as the Euclidean difference between that optimal trading position and the trading strategy that was actually executed. This difference is calculated taking into account all prices and traded quantities within the considered time window. The most important property of this approach is that it is completely objective i.e., we are capturing the impact caused by our own trading as a cost that affects all trades including our own and thus avoid the main problem with VWAP in the case of a large trading order. We discuss the properties of the new performance measure on real

trade data and demonstrate its main characteristics.

Analysis of a variational model for liquid crystal shells

Marco Veneroni

Abstract

We analyse an elastic surface energy which was recently introduced by G. Napoli and L.Vergori to model thin films of nematic liquid crystals. We show how a novel approach in modeling the surface's extrinsinc geometry leads to considerable differences with respect to the classical intrinsic energy. Our results concern three connected aspects: i) using methods of the calculus of variations, we establish a relation between the existence of minimizers and the topology of the surface; ii) we prove, by a Ginzburg-Landau approximation, the well-posedness of the gradient flow of the energy; iii) in the case of a parametrized torus we obtain a stronger characterization of global and local minimizers, which we supplement with numerical experiments. (Joint work with A. Segatti and M. Snarski.)

Spacetime Models of Gravity in Geolocation and Acoustics

Post-Newtonian Effects in Geolocation by FDOA

Jose Maria Gambi, Michael M. Tung, Javier Clares and Maria Luisa Garcia Del Pino

Author keywords: Geolocation, FDOA, Earth post-Newtonian framework.

Abstract

The post-Newtonian terms included in the FDOA equation derived by means of Synge's world-function are considered to estimate their contribution in the precise Geolocation of passive radio transmitters at rest on the earth surface. Four of these terms are kinematical and the other two are gravitational. The kinematical terms account for the velocities of the radio transmitter and the receivers with respect to the ECI reference frame, as well as for the relative velocities of the transmitter with respect to the receivers. The other two account for the gravitational attraction of an spherical earth on the receivers. The gravitational time delay has been taken into account to derive these terms.

Maxwell's Fish-Eye in (2+1)D Spacetime Acoustics

Michael M. Tung, José María Gambi and María Luisa García Del Pino

Author Keywords: spacetime models, transformation acoustics, differential geometry, Riemannian geometry, variational principle, Helmholtz equation.

Abstract

In the past few years Maxwells fish-eye lens has been subject to intense investigation in the context of transformation optics, mainly spurred by the possibility to create perfect imaging without the need to resort to negative refraction, one of the outstandingbut difficult to implementproperties of metamaterials. Here we extend this discussion to an acoustical fish-eye constructed in (2+1)D spacetime. The underlying acoustic wave is governed by a homogeneous spherical Helmholtz equation, which is shown to emerge from a variational principle in inherently covariant manner. The formal analytical solutions of the acoustic potential are derived.

Post-Newtonian Geolocation of Passive Radio Transmitters by TDOA and FDOA

Jose Maria Gambi, Javier Clares and Maria Del Carmen Rodriguez Teijeiro

Author Keywords: Geolocation, TDOA, FDOA, Earth post-Newtonian framework

Abstract

Different satellite configurations are considered to show by numerical simulations the influence of the post-Newtonian corrections to the standard location of radio transmitters by TDOA on the solution of the post-Newtonian FDOA equations. The satellites considered are LEO and GEO satellites in a number never smaller than five. The radio transmitters are supposed to be passive and are placed either on the earth surface or in space.

Post-Newtonian Orbital Equations for Fermi Frames in the Vicinity the Earth

Jose Maria Gambi, Maria Luisa Garcia Del Pino and Michael M. Tung

Author keywords: Geodesic deviation, APT systems, Earth post-Newtonian framework.

Abstract

Synge's equations for time-like geodesics in terms of Fermi coordinates are used to derive post-Newtonian equations for the relative motion of satellites in coplanar circular near orbits about the earth. The reference frame, co-moving with the base satellite, is assumed to be a Fermi frame, that is, inertial guided. The resulting system is autonomous, linear, and reduces to the equation of the geodesic deviation for nearby satellites. Hence, it can be used by some APT systems to increase the accuracy presently reached in locating passive radio-transmitters.

Imaging and inverse problems

Imaging in an optically thin media using L1-optimization

Pedro Gonzalez Rodriguez, Arnold D. Kim and Miguel Moscoso

Author Keywords: Radiative Transfer Equation, Optical tomography, L1-optimization

Abstract

We study optical imaging of a turbid medium in the mesoscopic scattering regime for which the thickness of the domain is just a few transport mean-free paths. For that case, light multiply scatters, but is not fully diffusive. Consequently, boundary measurements still contain angular information useful for reconstructing absorbing inhomogeneities in the medium. By considering measurements with different numerical apertures modeled by the Born approximation, and an 1-optimization method, we show that we can reconstruct absorbing inhomogeneities in tissues well.

Domain and parameter reconstruction in photothermal imaging

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Abstract

Photothermal imaging aims to reconstruct the inner structure of materials by heating their surface using a laser beam and recording the surface temperature. The goal is to detect structural defects or inclusions (determine their location, size, shape, orientation) and their nature (physical parameters).

In this work we propose an interative descent method that combines topological derivative computations to reconstruct the geometry of the defects with gradient iterations to approximate the material parameters.

Some numerical experiments showing the ability of the method to obtain reasonable reconstructions in a few iterations will be shown. Furthermore, we numerically corroborate that a small number of sampling points and source points allow for reliable reconstructions if we record the temperature during a time interval.

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Transmission eigenvalues for a dielectric object resting on a perfect conductor

P. Monk[72] and V. Selgas [73]

Abstract

We introduce a new transmission eigenvalue problem with mixed boundary conditions which arises when a dielectric scatterer is mounted on a metal structure. We describe the forward problem and show that it has a unique solution using a reflection principle. We also formulate the inverse problem of identifying the shape of the dielectric from near field measurements. To solve numerically this inverse problem, we propose the standard near field Linear Sampling Method (LSM); notice that the equations involved in the LSM and in the approximation of transmission eigenvalues from measurements are one and the same. Next, we reformulate the mixed transmission eigenvalue problem as a fourth order partial differential equation. Then we show that there exist infinitely many transmission eigenvalues and derive monotonicity as well as a lower bound estimate for the first eigenvalue. Our analysis mainly uses techniques from [4, 1, 1], and requires us to prove suitable density and compactness properties. We also provide numerical examples for the LSM; and finally demonstrate that, for the cases we have

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considered, mixed transmission eigenvalues can be approximated from near field data; see [3] for a study of the corresponding far field problem for standard transmission eigenvalues.

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Variational Models and Numerical Algorithms for one-dimensional Signal Reconstruction of Noisy and Blurry Signals: Application to the signal recovery for future detection of Gravitational Waves

Antonio Marquina, Alejandro Torres, Jose Antonio Font and Jose Maria Ibañez

Author Keywords: Total variation, denoising, l1-minimization, regularization, gravitational wave signals, bursts, chirps, Gaussian noise, convex energies.

Abstract

In this research work we examine the one dimensional variational models for reconstruction of signals using l1-Regularization. We present an analysis of the variational models based on l1-regularization and we implement numerical algorithms that allow to recover noisy and blurry signals, using direct methods and regularization procedures. We shall present an application for the recovery of one-dimensional signals to be observed in the near future in different gravitational wave detectors. In particular, we focus on a method for denoising and detection of gravitational waves embedded in additive Gaussian noise. The method is based on Total Variation denoising algorithms. These algorithms, which do not need any a priori information about the signals, have been developed and fully tested in the context of image processing. We apply our method to two different types of numerically-simulated gravitational wave signals, namely bursts produced from the core collapse of rotating stars and chirps from binary black hole mergers. First, we test the algorithms with some basic signals, in order to understand their properties and implement possible improvements. Next, we explore the parameter space of the method to find the set of values best suited for denoising gravitational wave signals. Finally, we apply our method to detect signals in a low signal-to-noise ratio scenario without any a priori information, to illustrate how this technique could be used simultaneously with other common techniques in gravitational wave data analysis to achieve detection.

Source reconstruction from final data in the heat equation

B. Tomas Johansson

Author Keywords: Inverse Problem, Heat Equation, Source Term, Regularization

Abstract

We consider the inverse ill-posed problem of determining an unknown source term in the linear heat conduction equation from final time data (together with known boundary and initial conditions) having applications in pollutant source identification and in the design of melting and freezing processes. We shall review a recent extension of a uniqueness result for source reconstruction. Moreover, an iterative method together with some numerical results for the reconstruction of a source from final data will be given.

The regularized split Bregman method based on rational approximations of the absolute value function for total variation image restoration

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The class of $l1-$regularized problems includes some relevant problems in computer science and imaging science. The Rudin-Osher-Fatemi (ROF) convex energy model defined as

$$\min_u \|\nabla u\|_1 + \frac{\lambda}{2}\|u - f\|_2^2$$

where f is the observed data or signal and $\lambda > 0$, is an important example of an efficient nonnegative functional for denoising signals or images. The $l1$-norm of the gradient, (total variation (TV) norm), is involved as regularizer of the ROF energy in order to preserve *edges* and avoid *ringing* in the solution u of the minimization problem. TV-based image denoising was first introduced in [2]. The ROF energy has been proved to be very difficult to minimize by means of standard methods. In [2] the authors used the gradient projection method which due to the non-differentiability of the

TV-norm behaved very slow and ill-conditionned. Fixed point iteration and primal-dual procedures have been designed to improve the efficiency of the minimization. Among many algorithms designed for solving the ROF model, Bregman iteration (introduced in [3], based on an iteration originally studied in [1]), has been shown very satisfactory. More recently, the Split Bregman procedure, ([4]), becomes an efficient algorithm where the $l1-$minimization is decoupled from the quadratic one using the evaluation of the *shrinkage* function.

In this research work we explore the regularization of the *shrinkage* function based on an approximation of the absolute value function to design a class of Split Bregman methods for TV image restoration. We introduce a hierarchy of regularizations depending on a positive parameter that determines the accuracy in the approximation of the absolute value function by means of rational functions. According to the order of the approximation of the generating rational function used, the degree of *smoothness* can be dosed for particular image processing applications.

We use appropriate rational real functions $R(x)$ that approximates the function $|x|$ uniformly in $[-1; 1]$ (as proposed in [5]) to approximate the nonlinear *shrinkage* functions scaled by an upper bound of the magnitude of the gradient. We study different rational approximations: Newman-type functions, iterative generated Halley functions and also Chebyshev polynomial approximants. We present a set of numerical tests involving the restoration of signals and synthetic images contaminated with noise and blur.

This research work was made in collaboration with Antonio Marquina, Universitat de Valencia (Spain).

Minisymposium: Imaging and Inverse Problems

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Fast Backprojection Operator for Synchrotron Tomographic Data

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Reduction of computational time in high resolution image reconstruction is essential in basic research and applications as well. This reduction is important for different types of traditional non diffractive tomography in medical diagnosis as well as for applications in nanomaterials research, related to modern technologies. Alternatives to alleviate the computationally intense part of each iteration of iterative methods in tomographic reconstruction have all been based on interpolation over a regular grid in the Fourier domain or in fast nonuniform Fourier transforms. Both approaches speed up substantially the computation of each iteration of classical algorithms, but are not suitable for being used in a large class of more advanced faster algorithms: incremental methods such as OS-EM, BRAMLA or BSREM, among others, cannot benefit from these techniques.

The backprojection is a stacking operator, known as the adjoint of the Radon transform. As a mapping $\mathbf{B} : g \to b$, acting on a sinogram $g = g(t, \theta)$, it is defined as

$$b(x) = \mathbf{B}g(x) = \int_0^\pi g(x \cdot \xi_\theta, \theta) d\theta, \quad \xi_\theta = (\cos\theta, \sin\theta), \quad x \in \mathbb{R}^2$$

It can be shown that $\mathbf{B}$ can be recasted as a convolution operator, in a different coordinate system, which is an obvious improvement in acceler-

[74]Second author supported by FAPESP grant No 2013/16508-3

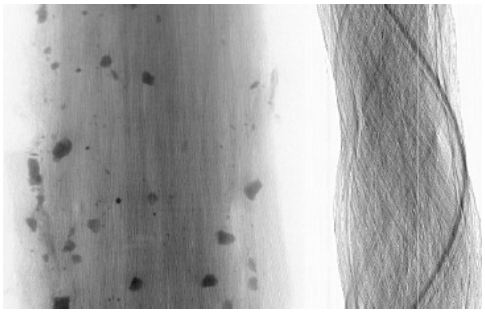

Figure 1: Left: typical projection of a given sample. Right: sinogram g extracted from projections.

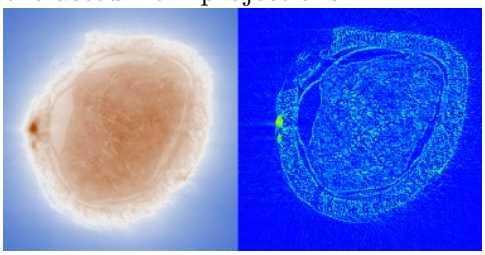

Figure 2: Left: backprojection function $b = \mathbf{B}g$. Right: Filter of the function b.

ating the computation of $\mathbf{B}$. In this work, we propose several analytical representations for the operator $\mathbf{B}$, in order to find a fast algorithm for the computation of the function $\mathbf{B}g$.

Computational Finance

Portfolio optimization in the case of an asset with a given liquidation time distribution

Ivan Yamshchikov, Ljudmila Bordag and Dmtry Zhelezov

Author Keywords: portfolio, optimization, illiquidity, viscosity solutions, random income

Abstract

Management of the portfolios containing low liquidity assets is a rather tedious problem. The buyer proposes the price that can differ greatly from the paper value estimated by the seller, the seller, on the other hand, can not liquidate his portfolio instantly and waits for more favorable offer. To minimize losses in this case we need to develop new methods. One of the steps moving the theory towards practical needs is to take into account the time lag of the liquidation of an illiquid asset. This task became especially significant for the practitioners in the time of the global financial crises.

Working in the Merton's optimal consumption framework with continuous time we consider an optimization problem for a portfolio with an illiquid, a risky and a risk-free asset. While a standard Black-Scholes market describes the liquid part of the investment the illiquid asset is sold at a random moment with prescribed liquidation time distribution. In the moment of liquidation it generates additional liquid wealth dependent on illiquid assets paper value. The investor has the logarithmic utility function as a limit case of a HARA-type utility. Different distributions of the liquidation time of the illiquid asset are under consideration - a classical exponential distribution and Weibull distribution that is more practically relevant. Under certain conditions we show the existence of the viscosity solution in both cases and study possible reductions of an exponential case using Lie group analyses. Applying numerical methods we compare classical Mertons strategies and the optimal consumption-allocation strategies for portfolios with different liquidation-time distributions of an illiquid asset.

A Positive, stable and consistent front-fixing numerical scheme for American Options

Rafael Company, Vera Egorova and Lucas Jódar

Author keywords: Finite difference scheme, Free boundary, Stability, Consistency, Positivity.

Abstract

In this paper we propose an explicit finite-difference scheme to solve the American option pricing problem. It is based on front-fixing transformation that involves unknown free boundary to the equation. The proposed stable and consistent numerical scheme preserves positivity and monotonicity of the solution in accordance with the behavior of the exact solution. Numerical examples and comparison with other methods are included. This technique can be applied to some types of two-asset options after reducing of the dimension. In the paper the front-fixing method is applied to exchange option pricing.

Numerical Solution of Partial-Integro Differential Option Pricing Models with Cross Derivative term.

M. Fakharany, R. Company and L. Jódar[75]

Abstract

The aim of this paper is to construct a reliable and efficient finite difference scheme for American option pricing under Bates model. First, we transform the associated partial-integro differential equation for this model into another suitable one without the cross derivative. Thereafter, a finite difference discretization has been used for the partial derivatives while the integral part is discretized using the four-points open type formula. The obtained finite difference scheme is solved using PSOR method. Several examples are included showing the advantage of the proposed approach.

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An efficient Monte Carlo algorithm for pricing arithmetic Asian options under a jump diffusion process

Walter Mudzimbabwe

Abstract

We develop a Monte Carlo algorithm to price an Asian option whose underlying price is driven by a jump diffusion process. By conditioning on the number of jumps, we are able to characterise the price process as lognormally distributed from which a control variate for the generic Monte Carlo algorithm is derived. Numeric results confirm that the control variate method is an effective variance reduction method.

Option pricing in exponential Levy models with transaction costs

Nicola Cantarutti

Abstract

The aim of this work is to extend the model of Barles and Soner for the option pricing with transaction costs. In a market with transaction costs, there is not a portfolio that replicates a european call option. For this reason, it is necessary to relax the hedging condition, requiring the portfolio only to dominate, rather than replicate, the value of the option. But doing super-replication with the presence of transaction costs turn out to be too costly. So the method of Barles and Soner is to introduce preferences, following the utility function approach of Hodges and Neuberger. Starting from a singular stochastic control problem, they study the asymptotic behaviour of the solution of the Hamilton-Jacobi-Bellmann equation, when the number of options goes to infinity and the transaction cost goes to zero. They derive a non-linear Black-Scholes equation for the price of the option with an adjusted volatility which is a function of the second derivative of the price itself. In this model, the dynamics of the underlying asset follows the geometric brownian motion. It is well known that this is an unrealistic representation of the real market dynamics. So the goal is to replace this price dynamics with a more general exponential Levy process. This has the effect of modifying the initial stochastic control problem as well, because the new HJB equation has an additional integral term. We show a comparison between the Barles and Soner equation with the new PIDE. We further present some numerical results for the option pricing with transaction costs.

Analysis of a Cross-Diffusion Herding Model in Social Economics

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Modern psychological and economic research has identified herd behavior in humans to explain phenomena of large numbers of people acting in the same way at the same time.

We model information herding in a macroscopic setting by analysing the following cross-diffusion model

$$\begin{cases} \partial_t u = div(d_1 \nabla u - \chi g(u) \nabla u) \\ \partial_t v = div(\delta \nabla u - \kappa \nabla v) + f(u) - \alpha v \end{cases}$$

with no-flux boundary conditions and initial conditions in a bounded domain $\Omega \in \mathbb{R}^d$ with $d_1, \chi, \kappa, \alpha > 0$ and $\delta \in \mathbb{R}$.

The function u depends on x and t. We consider x as a multidimensional information variable (political opinion, wealth of individual or company...), and, as usual, t is the time. We may interpret u as an information density which represents the number of people having the information x at time t and it is influenced by the potential v which expresses the tendency of people to adapt their individual opinion to the majority opinion.

If $\delta = 0, g(u) = u(1-u), f(u) = u$ or $f(u) = u(1-u)$ the system models the crowd motion and herding [1, 2]. The global existence of solutions to the system for the choices $g(u) = u$ and $g(u) = u(1-u), \delta = 0$ has been already shown, under some appropriate additional conditions in [5]. The term $g(u) = u(1-u)$ forces the information density to attain values in

the interval $[0,1]$. However, the system with $\delta = 0$ does not possess an entropy structure which complicates the analysis of the long-time behavior. Therefore, we suggest to include the regularizing term $\delta\Delta u$. This term allows for an entropy structure useful for the mathematical analysis and introducing an additional modeling parameter. If $\delta > 0$ and the functions f and g are chosen in an appropriate way, the above system possesses an entropy functional and we can prove the global existence of weak solutions as have done in [3], and we can study the long-time behavior. In particular we are interested in studying under which condition there is congestion, i.e. we have existence of non-constant steady states. With this aim, we are trying to apply the bifurcation theory (see [4]) in order to understand the behavior of the solutions.

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A boundary element method for pricing barriers options

Chiara Guardasoni and Simona Sanfelici

Author Keywords: Boundary Element Method (BEM), Barrier Option, Heston model

The study of phenomena modeled by boundary value problems for partial differential equations is wide in Physics and Engineering but also in Finance and Economics in general. From 1970s, with the introduction of the electronic computers, Boundary Element Method (BEM) has been largely used and improved in Physics and Engineering and in particular, more recently, its application has been refined for time-dependent problems that involve more difficult theoretical analysis. Despite this, only the very recent contribute by Ballestra ([1]) is available in literature about its application to Quantitative Finance. BEM is a method for partial differential equations in which a reduction in mesh dimension from a domain-type to a boundary-type is accomplished. The advantages of BEM, when compared to domain methods, such as Finite Element Methods (FEM) or Finite Difference Methods (FDM), are well known: only the boundary of the domain needs to be discretized, particularly, exterior problems with unbounded domains but bounded boundaries are handled as easily as interior problems. Therefore, this feature makes this method pretty interesting when considering options with single/double barriers: the solution in the domain is approximated with a rather high convergence rate and can be evaluated at particular points of the domain and not necessarily everywhere on a defined grid; infinity conditions are implicitly satisfied. Note that, for plain vanilla options, BEM reduces to the traditional Green's function approach, i.e. the computation of the option price as discounted expectation of the final payoff under suitable probability measure. One of the main difficulties that could arise applying

this method, concerns the necessary explicit knowledge of a fundamental solution for the differential equation that is generally available only for linear partial differential equations with constant or some specific variable coefficients. The fundamental solution is available in Black-Scholes case but, when considering more complicated models with stochastic volatility (such as Heston model [4]) and jumps (as in Bates model [2]), only the Fourier transform of the fundamental solution is known, so a good strategy has to be carried out to overcome this complication. For Black-Scholes equation, BEM is really efficient and accurate as already deeply investigated in [1] and [3], where the authors have tested the method for different types of barrier options. Here, we will show that this method maintains these qualities also when we don't rely on the analytical expression for the fundamental solution.

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A class of nonlinear boundary value problems for a Black-Scholes type equation

Rubén Figueroa and Maria Do Rosário Grossinho

Author Keywords: Nonlinear Black-Scholes-type equation, Transaction costs, Upper and lower solution method.

Some generalizations of the classical Black-Scholes model that incorporate the effects of transactions cost when hedging a portfolio lead to the study of nonlinear differential equations. Leland (1985) suggested a market with proportional transaction costs. We consider a model where the transaction costs are not proportional to the amount of the transaction but the individual cost of the transaction of each share diminishes as the number of shares transacted increases. This leads to a partial differential equation that contains the terms of the classical Black-Scholes equation, an additional nonlinear term modeling the presence of transaction costs, and an adjusted volatility. We are concerned with the existence of convex stationary solutions for boundary value problems from this Black-Scholes-type PDE and generalize the results contained in Amster, Averbuj, Mariano and Rial (2005), and Grossinho and Morais (2009, 2013). In fact, we consider a variable volatility and abstract functional boundary conditions, which allows us to treat a very large class of problems involving Black–Scholes equation. Our main results involve the existence of extremal solutions in presence of lower and upper solutions. Some examples are provided, too.

Derivative pricing with transaction costs using a stochastic utility maximization model

Daniel Ševčovič, Manuel Guerra and Pedro Pólvora[76]

Abstract

The pricing of financial derivatives with transaction costs is one of the most important extensions of the traditional Black-Scholes model. Stochastic utility maximization models can be used for the pricing of derivatives under these conditions, in this type of models the price is found by computing the certainty equivalent of the portfolio with the option and compare it with the certainty equivalent of the portfolio without the option.

One of the most well-known models of this kind was developed by Barles and Soner in 1998, it includes proportional transactions costs and considers an exponential utility function, they use it to price an European Call option. In this paper we present a study on the extension of the model developed by Barles and Soner in terms of a broader type of utility functions (such as HARA-type utility functions) and derivatives payoffs.

We make use (as in the original model) of the stochastic dynamic programming principle to find the set of HJB equations whose solution will represent the certainty equivalent of both portfolios. The price of the deriva-

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tive will be given by the difference of those two functions. We compare the solutions with the original model in particular in terms of the asymptotic analysis of these equations.

Extension of a Fourier-cosine method to solve BSDEs with higher dimensions

C. W. Osterlee and M. Pou[77]

Abstract

A Backward Stochastic Differential Equation (BSDE) is a stochastic differential equation for which a terminal condition has been specified. In [6] a Fouriercosine method to solve BSDEs is developed. This technique is known as BCOS method and consists of the approximation of the BSDEs solution backwards in time by the use of the COS method developed in [2] to compute the conditional expectations that rise after the discretization by means of a q-method for the timeintegration. In our work, this methodology is extended to the case in which the terminal condition depends on more than one process, allowing that the pricing of derivatives contracts such as rainbow options. The extension of the BCOS technique can be done taking into account some ideas developed in [5]. We present some numerical examples concerning to derivatives on two processes without jumps. We also apply our extended method to solve the BSDEs that rise with the use of quadratic hedging techniques for pricing in incomplete markets without or with jumps [3,4]. Problems in which the randomness of the terminal condition is origi-

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nated not only from the risky asset but also from the insurance risk or the counterparty default risk can be introduced in this framework [1].

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Fichera theory and its application in finance

Zuzana Bčková, Matthias Ehrhardt and Michael Günther[78]

Abstract

The Fichera theory was first proposed in 1960 by Gaetano Fichera [1] and later developed by Olejnik and Radkevič in [3]. It turned out to be very useful in clarifying questions of well-posedness for a wide range of partial differential equations. The sign of the so-called Fichera function clarifies whether we have to impose boundary conditions in a finite difference scheme or not.

In this work we present some application of the Fichera theory to interest rates models of Cox-Ingersoll-Ross (CIR) and Chan-Karolyi-Longstaff-Sanders (CKLS) type. For the one-factor CIR model the obtained results are consistent with the corresponding Feller condition.

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High-order compact finite difference schemes for parabolic differential equations with mixed derivative terms in n space dimensions and application to basket options

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Abstract

In this talk we derive and analyse a high-order compact scheme for partial differential equations with mixed derivative terms in n space dimensions of the form

$$u_t + \sum_{i=1}^{n} a_i \frac{\partial^2 u}{\partial x_i^2} + \sum_{i,j=1, i<j}^{n} b_{i,j} \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^{n} c_i \frac{\partial u}{\partial x_i} = d \quad \text{in } \Omega \times \Omega_\tau \qquad (3)$$

with initial condition $u_0 = u(x_1, \ldots x_n, 0)$. We have $\Omega \subset \mathbb{R}^n$ as an $n-$dimensional rectangle and $\Omega_\tau =]0, \tau_{max}]$ with some $\tau_{max} > 0$. Additionally the coefficients $a_i (< 0), b_{ij}, c_i$ and d are functions of $(x, \tau) \in \Omega \times \Omega_\tau$ for $i, j \in \{1, \ldots, n\}$.

We derive conditions on the coefficients of (3) under which it is possible to obtain fourth-order accuracy in space in terms of the stepsize $h > 0$, where $\Delta x_i \in O(h)$ for all j, and second-order accuracy in time for a Finite Difference scheme on the compact stencil. This leads to overall convergence order of four in terms of h if $\Delta\tau \in O(h^2)$.

As a next step we perform a von Neumann stability analysis for spatial domains with dimensions two and three for frozen coefficients, where we prove that a necessary stability condition holds unconditionally without additional restrictions on the choice of the discretisation parameters for vanishing mixed derivative terms. We also give partial results for non-vanishing mixed derivative terms.

As example Black-Scholes Basket Power options are considered. As the convergence rate of a numerical scheme is limited by the smoothness of the initial condition, we use the smoothing operators of Kreiss, Thomee, and Widlung to smoothen the intial conciditon for the power options. In all numerical experiments a comparative standard second-order discretisation is significantly outperformed.

Efficient calibration and pricing in LIBOR Market Models with SABR stochastic volatility using GPUs

A. M. Ferreiro, J. A. García, J. G. López-Salas and C. Vázquez[79]

Abstract

In this work we study three extensions of the LIBOR market model (LMM) [1] that reproduce for all strikes and maturities the prices of plain vanilla instruments (caplets and swaptions) produced by the SABR stochastic volatility model [5]. The SABR model has become the market standard to interpolate and extrapolate prices of plain vanilla caplets and swaptions. It is widely used because it yields to a closed-form formula for the implied volatility which allows an easy calibration of the model. LMM joins all the forward rates under a single measure, so that it specifies dynamics simultaneously valid for all the underlyings. Therefore it allows to price complex instruments. However, its main drawback is the use of constant volatilities. SABR/LIBOR market models combine the advantages of these two models. We have considered the SABR/LIBOR models proposed by P. Hagan [4], F. Mercurio & M. Morini [6] and R. Rebonato [7]. The efficient calibration to market data of these models becomes a relevant target in practice.

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In general, swaptions cannot be priced in closed form in the LMM and the main challenge of the previous works comes from the analytical approximations to price them. They argue that the *brute-force* approach, which consists in calibrating the models using Monte Carlo evaluation to price swaptions, is not a practical choice, because each Monte Carlo evaluation results computationally very expensive. However, in this work we propose a parallelized version of the simulated annealing algorithm for multi-GPUs that makes possible this approach in reasonable computational time. The numerical results illustrate the advantages of using the proposed multi-GPUs tools when applied to real market data and the three SABR/LIBOR models. Such algorithms have already been successfully applied in other related contexts, see [2, 3] for more details.

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Numerical solution of stochastic PDEs arising in financial engineering

Christoph Reisinger

Author Keywords: stochastic PDEs, large particle systems, multilevel Monte Carlo simulation, variance reduction.

The talk focuses on the estimation of expected functionals of the solution to certain stochastic partial differential equations of parabolic type. These SPDEs arise in diverse situations, in particular describing the empirical measure of a large pool of assets, and the evolution of expected option payoffs conditional on stochastic parameters. In the main part of the talk we present a multilevel Monte Carlo simulation method and analyse its convergence properties. Numerical results are discussed for an application from basket credit derivatives and for a variance reduction method based on a hybrid simulation of conditional expectations.

A Fokker-Planck Strategy to Control Stochastic Processes[80]

M. Annunziato[81] and Alfio Borzì[82]

Abstract

An efficient framework for the optimal control of probability density functions (PDF) of multidimensional stochastic processes and piecewise deterministic processes is presented. This framework is based on Fokker-Planck-type equations that govern the time evolution of the PDF of stochastic processes. In this approach, the control objectives may require to follow a given PDF trajectory or to minimize an expectation functional. Theoretical results concerning the forward and the optimal control problems are provided. In the case of stochastic (Ito) processes, the Fokker-Planck equation is of parabolic type and it is shown that under appropriate assumptions the open-loop bilinear control function is unique. In the case of piecewise deterministic processes (PDP), the Fokker-Planck equation consists of a first-order hyperbolic system. Discretization schemes are discussed that guarantee positivity and conservativeness of the forward solution. The proposed control framework is validated with multidimensional biological, quantum mechanical, and financial models.

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Modelling Stochastic Correlation

Long Teng, Matthias Ehrhardt and Michael Günther[83]

Abstract

This chapter deals with the modelling of correlation. It is well known that the correlation between financial products, financial institutions, e.g., plays an essential role in pricing and evaluation of financial derivatives. Using simply a constant or deterministic correlation may lead to correlation risk, since market observations give evidence that the correlation is not a deterministic quantity.

In this chapter, we describe a new approach to model the correlation as a hyperbolic function of a stochastic process. Our general approach provides a stochastic correlation which is much more realistic to model real world phenomena and could be used in many financial application fields. Furthermore, it is very flexible: any mean reverting process (with positive and negative value) can be regarded and no additional parameter restrictions appear which simplifies the calibration procedure. As an example, we compute the price of a quanto applying our new approach. Using our numerical results we discuss concisely the effect of considering stochastic correlation on pricing the quanto.

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Mathematical Modelling in Energy Markets

Valuation of Storage Contracts in Incomplete Gas Markets

Magnus Wobben

Author keywords: Optimal hedging in incomplete markets, Valuation of gas storage contracts, Risk aversion

Abstract

Hedging against price and volume uncertainties in incomplete gas markets has recently become an important issue for both practitioners as well as academics. Accordingly, various types of contracts with flexible structures, such as physical and virtual gas storages show increasing trading volumes. However, due to their complex nature together with the markets' incompleteness, valuation and hedging of these contracts is non-unique and challenging. In this article, we present a universal and practical framework that overcomes the fallacies of incomplete markets and gives a market-coherent and efficient valuation of gas storage contracts.

Integrated Forecasting of day-ahead Prices in the German Electricity Market

Christian Hendricks, Matthias Ehrhardt and Michael Günther[84]

Abstract

Since the start of the liberalization of energy markets the energy sector has undergone major changes. Energy companies now provide electricity at variable prices and are faced to a competitive market environment. Their trading is subject to risks and uncertainty about future price developments. These risks are mainly associated with the volatile nature of input costs, like coal and gas prices. In this paper we introduce a regularized regression approach to forecast *Phelix Peak* prices in the German electricity market. Additionally we investigate the influence of fundamental price drivers on the forecasting accuracy. Since the problem complexity grows exponentially with the dimension of the feature space, the regression problem suffers from the curse of dimensionality. To cope with this problem we apply the combination technique. It is based on a linear combination of coarse grids to the so called sparse grid solution, which enables us to reduce the complexity but keep a high approximation accuracy.

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Nonparametric modelling and short-term forecasting of French electricity demand and spot prices

Virginie Dordonnat and Yannig Goude

The aim of the talk is to present an overview of what has been achieved regarding GAM modelling of electricity demand, whether on the aggregate (national) or local level. We will also present a more recent application for the short-term forecasting of spot prices.

An Introduction to Mathematical Models in Energy Markets

Michael Coulon

Author Keywords: energy, price, modeling, markets, electricity, finance.

How much benefit can mathematical or statistical models bring to real-world challenges in energy markets? As the field has grown and gained much attention in recent years, we believe that the answer is a lot! However, it is important to understand the limitations of the models as well as their advantages. Energy markets (and electricity markets even more so) require considering a wide range of factors, risks, and phenomena not seen in other markets. How can we best adapt traditional techniques from mathematical finance to meet these challenges, or should we just start from scratch? There are many interesting questions in energy markets, often relatively little consensus, and much room for innovative modeling ideas. We provide an introduction to mathematical modeling of energy prices by reviewing the approaches most commonly used (with particular focus on electricity markets as a complex challenge), analyzing their strengths and weaknesses, and discussing goals and challenges for the future.

Optimizing renewable, hydro and gas assets as realistically as possible

Christian Jacobsson

Author Keywords: dynamic programming, stochastic dynamic programming, neural network, optimization, hydro, gas, renewable, wind, solar.

Assets need to be operated daily, and an optimization taking uncertainties into account is needed to maximize profits and to handle risks. We make an attempt to optimize the assets as realistically as possible with respect to plant specifications, stochastic elements and market liquidity, using stochastic dynamic programming. We also try to curb the curse of dimensionality of flexible hydro asset optimization using approximate dynamic programming, representing the value-function by a neural network with built-in function knowledge.

Explaining gas storage levels using price information

Alexander Boogert

Author Keywords: gas storage, volume level, simulation based optimization.

One of the principles behind gas storage valuation is that a gas storage owner can react to changing gas prices, and thus capture value from the flexible asset. In the literature several methods have been proposed to price and hedge individual gas storages. In this view a gas storage level is a consequence of following a certain optimization strategy.

Due to recent regulation, gas storage operators in Europe are starting to publish gas storage levels on an individual basis. In this talk we study such data and consider the question whether we can explain these storage levels. We test whether it is possible to explain storage levels looking at price levels in the market. In particular, we consider what happens if we do not have access to the underlying trades in the forward market of the operator, and can only observe the daily volumetric changes.

Currency Risk in Energy Markets

Nina Lange

Author Keywords: Energy Markets, Currency Risk, Correlation.

An investor in commodity markets are faced with both price risk and currency risk, as the commodity is often traded in a different currency than the investor's own. Often, the news report that the commodity prices and the USD/EUR rate move in opposite directions, indicating that the currency risk and price risk offsets each other for a Euro denominated investor. In this paper, I investigate if this is in fact the case and to which extent the correlation connects to the volatility of the commodity price and exchange rates. The paper introduces a model which allows for stochastic correlation of both signs and models the futures price curves and option prices in a model. The model is estimated using data on WTI crude oil and EURUSD futures contracts traded at the Chicago Mercantile Exchange from 1998 to 2013.

Industrial Particle and Interface Dynamics

The generation and interaction of convection modes in a box of a saturated porous medium.

Brendan J. Florio

Abstract

Convection in an infinite layer of porous media occurs if the dimensionless Rayleigh number exceeds a critical value. This is also true for a box of porous media, however, each discrete modal solution has its own associated critical Rayleigh number. Usually just one mode will be generated at the onset of convection, however, there are many critical box dimensions for which up to four modes share the same critical Rayleigh number and all may be generated at the onset of convection. In such circumstances there will be a slow interchange of energy between the preferred modes. A perturbation method is applied to a system where three modes are generated at onset to yield a system of ordinary differential equations which govern the evolution of the amplitudes of the viable modes. Three unique cases arise, each with a different phase-space structure. Critical boxes with *moderate* aspect ratios are are systematically categorised into these cases. While two of the examples represent the usual case where just one mode survives in the final state, the third example is a special case where it is possible for the three modes to coexist. The initial conditions determine which mode(s) will survive. For non-critical boxes, the bifurcations that occur as the Rayleigh number increases are analysed and profiled in the weakly-nonlinear regime.

Modelling particle-wall interaction in dry powder inhalers

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Abstract

Dry powder inhalers deliver drugs in powdered form to the lungs. The drug is stored within the inhaler bound to an excipient. The conglomerate is broken apart in a vortex chamber by collisions with the walls and other conglomerates. During the initial doses, some drug adheres to the wall of the vortex chamber reducing the amount of drug delivered to the patient. We developed mathematical models for particle-wall adhesion to investigate why drug particles adhere to the wall of the vortex chamber. Two different models are developed to validate our results and a good agreement has been obtained. The first model is a continuum model of particle-wall adhesion based on Partial Differential Equations (PDE). This model focuses on the rate at which drug particles are captured by the wall and the time taken for drug particles to fill the wall area. The second model describes the motion of particles in a flow field based on Stochastic Differential Equations (SDE). Estimates of magnitudes of adhesive forces suggest that excipient particles do not adhere to the walls, while drug particles bind to the wall due to van der Waals forces when their velocity is below a critical value. Drug adhesion is primarily affected by Hamaker constant, surface roughness and coefficient of restitution.

Optimising copying accuracy in holographic patterning

Dana Mackey, Izabela Naydenova and Paul O'Reilly

Author keywords: holographic gratings, photopolymer materials, perturbation methods, partial differential equations

Abstract

Recent advances in optical processing have contributed to the rapid growth of holography, with exciting applications to holographic sensors, recording devices and data storage. The successful implementation of these applications requires however more research into the design of the ideal photosensitive material for holographic recording.

It is known that exposing a photopolymer material to an illumination pattern causes light induced mass transport of the photopolymer components. The recorded holographic grating is then due to a spatial variation of the refractive index resulting from changes in the density of the monomer and polymer species. We propose a partial differential equations model for the formation and evolution of the holographic grating and use perturbation methods and numerical simulations in order to investigate the dynamical mechanism by which distortions of the illumination pattern arise during recording. The parameters of interest are diffusion and photopolymerisation rates as well as exposure time, for which we seek to determine regimes which allow for high fidelity copying. This study is first undertaken for a one-dimensional sinusoidal illumination pattern and then generalized to two-dimensional gratings created by multiple beam holography. An extensive geometrical study is necessary here for analysing the properties of the

lattice created by the interference of three beams and optimising the illumination intensity contrast. We find good agreement between theoretical and experimental data, for different geometries and conditions of exposure.

Mathematical Modelling of the Coffee Brewing Process

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The drip filter coffee market is a multi-billion euro industry. Despite this, although the chemistry of coffee brewing has been investigated in great detail, the physics of the process has received relatively little attention. In order to explain in scientific terms correlations between the coffee quality and the process variables a physical model is required. In this study, flow through a static, saturated coffee bed, under the in uence of a pressure gradient, is described using a double porosity model. The model is parametrised using experimentally obtained data from a cylindrical flow-through cell containing a coffee bed. Mass transfer from the coffee grains to the interstitial water is modelled using two mechanisms; mass transfer from the surface of the grains and mass transfer from the interior (bulk) of the grains. Mass transfer resistances are estimated by fitting experimental data. Initially coffee extraction is dominated by mass transfer from the grain surface, while transfer from the kernel of the grain is the rate limiting mechanism once the surface coffee has been exhausted. The model is non-dimensionalised to identify the timescales of these processes, allowing model reduction based on the dominant mechanisms and approximate solutions to be developed. Numerical and approximate solutions are compared with experimental data.

Numerical analysis and simulations of a mixed kinetic-diffusion model for surfactant solutions

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Author Keywords:surfactant, diffusion, adsorption-disorption, kinetic-diffusion model, finite element method, simulations

The behavior of surfactant solutions at the air-water interface plays an important role in several biological, biochemical and industrial processes. When a new surface is formed in a surfactant solution, the surfactant molecules tend to migrate from the bulk of the solution to the air-water interface changing the surface properties, being one of the most important the dynamic surface tension.

From the mathematical point of view, the process is modeled by the diffusion partial differential equation in one spatial dimension, together with suitable initial and boundary conditions, the unknowns being both the surface and the bulk concentrations. In order to close the problem, we must consider an adsorption model that is coupled to the system by means of the boundary condition at the subsurface. In this case, we take into account a mixed kinetic-diffusion model, and we focus on a modification of the Langmuir-Hinshelwood equation which is given by an ordinary differential equation.

For this nonlinear problem, we study the existence and uniqueness of a weak solution and we carry out the numerical analysis of a fully discrete approximation of the variational problem. This approach is obtained applying

the finite element method to approximate the spatial variable and a hybrid combination of both backward and forward Euler schemes to discretize the time derivative. Then, we obtain some a priori error estimates and, under additional regularity conditions, the linear convergence of the algorithm is achieved. Finally, we perform some numerical simulations in order to show the accuracy of the approximation and the behavior of the solution for some commercial surfactants.

Mathematical Modelling for Stout Beer Widgets

William Lee

Author Keywords: Bubbles, Nucleation, Cellulose.

Abstract

Technology for promoting bubble nucleation is important in designing engraved champagne glasses, siphons for degassing carbon dioxide saturated lakes and and stout beer widgets. The current generation of stout beer widgets relies on the generation of a large number of bubbles nuclei from the breakup of a turbulent jet of gas released from a pressurised ball. There are a number of disadvantages to this approach which it may be possible to overcome using widgets based on cellulose fibres. We report progress towards developing models of bubble nucleation by cellulose fibres that can be used to develop such a widget.

Robust Variable-Structure Approaches for Control and Estimation of Uncertain Dynamic Processes

Extension of Sliding Mode Observer for Fault Reconstruction: Comparsion between LPV and Takagi-Sugeno model approach

Horst Schulte and Soren Georg[85]

Abstract

This paper compares recently proposed fault reconstruction methods using sliding mode observer for a class of linear parameter varying (LPV) [2] with Takagi- Sugeno systems [3]. Both methods are an extension of a canonical form for sliding mode observer design, originally restricted to linear time invariant systems [1]. The methods are compared analytically and by simulation. The underlying relation between them is exposed.

In the last decades there has been an explosion of interest in the use of sliding mode methods for fault detection, isolation (FDI) and fault reconstruction using the equivalent output injection signal. The fault reconstruction can be exploited for fault tolerant control (FTC) in the sense that sensor and actuator faults are corrected before the measurement are used for the controller or rather the control signal acts on the plant. Originally the

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sliding mode method based on linear time invariant (LTI) systems with unknown but bounded terms [1]. An important extension to the sliding mode observer concept is to introduce a convex combination of LTI systems. The combination can be parameter-varying or state-varying with the constraint, that all output matrices are common. The parameter-varying concept was presented in [2] and based on a class of LPV systems. In contrast, the state-varying sliding mode concept was first proposed in [3], where the observer is implemented within a Takagi-Sugeno (TS) model structure to account for system nonlinearities. Both approaches proposed extensions of the LTI scheme of sliding mode observer to a convex combination of LTI systems, which is a suitable compromise between a full nonlinear design and the LTI framework.

In this paper differences and similarities between these methods were discussed in detail. The efficiency of the methods are investigated using two benchmark problems, the inverted pendulum and an aircraft problem from the literature.

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Experimental Validation of State and Parameter Estimation using Sliding-Mode Techniques with Bounded and Stochastic Uncertainty

Minisymposium: Robust Variable-Structure Approaches for Control and Estimation of Uncertain Dynamic Processes

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Uncertainties - more precisely bounded and stochastic disturbances - play a major role in control and estimation tasks in general. Examples for bounded uncertainty are lack of knowledge about specific parameters and manufacturing tolerances. Moreover, stochastic disturbances have a very important impact on dynamic systems, especially in sensor measurements. These issues make it difficult to control a system such that robustness and stability are guaranteed especially if system parameters are not exactly known and system states cannot be measured with high accuracy due to process and measurement noise. The mathematical description of the considered system including the most important deterministic characteristics

is essential for a combined state and parameter estimation. Therefore, a sliding mode observer that copes with uncertain parameters as well as with noisy measurements is proposed in this presentation. States and parameters are estimated in such a way that the error dynamics are stabilized. The advantages of the presented observer are robustness and stability based on the usage of suitable candidates for Lyapunov functions as it is usually done in existing sliding mode approaches. The differences to existing sliding mode observers are that, firstly, no restrictive matching conditions occur which, hence, lead to a more general applicability of the observer. Secondly, interval descriptions are used for uncertain states as well as parameters. Finally, modeling different kinds of nonlinearities that inevitably influence the stability of the system - as for example friction, wear of mechanic components or remanence of a brake - can be included as stochastic disturbances.

Considering interval arithmetic is in general useful if a system is affected by uncertainty that influences the system dynamics in an significant way. Therefore, not only intervals for parameters but also for measurement uncertainty and errors of the estimated states can be taken into consideration. The number of calculated switching amplitudes of the presented observer is equal to the number of measurements. This enables an individual computation of the switching amplitudes for the estimation of states and parameters according to the evaluation of a Lyapunov function using the Itô differential operator for stochastic processes. Moreover, Pontryagin's maximum principle is used for an optimal input design to improve the parameter estimation.

Simulation results show the practical applicability of this approach for estimating states and parameters. Numerical results of the parameter estimation using the sliding mode approach are compared with a least-squares parameter identification to point out the improved performance of the observer. For this comparison, experimental data from a test rig available at the Chair of Mechatronics at the University of Rostock are used.

Interval-Based Sliding Mode Control for High-Temperature Fuel Cells under Actuator Constraints

Minisymposium: Robust Variable-Structure Approaches for Control and Estimation of Uncertain Dynamic Processes

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In previous work, different approaches have been derived by the authors for the reliable control of the thermal behavior of high-temperature fuel cell stacks under consideration of uncertain parameters and not a-priori known load variations. These control approaches comprise model-predictive, feedback linearizing, and sliding mode techniques. It was shown that both the predictive and sliding mode techniques can be applied successfully to system models with interval parameters.

In contrast to the predictive control approach, physical state and actuator constraints cannot be handled directly within a classical sliding mode design for this type of application. However, the sliding mode-type control design provides an inherent stability proof, which is not directly available for the predictive technique. For these reasons, this contribution removes the before-mentioned drawback concerning the handling of constraints by a reformulation of the stability conditions resulting from the variable struc-

ture control design. This reformulation is based on a stability-preserving nonlinear gain adaptation scheme that is employed as soon as saturation limits are reached. For that purpose, actuator limits are treated as hard constraints that must not be exceeded under all circumstances. State limitations, however, are described by soft constraints. They are considered by corresponding weak penalty terms.

In such a way, it becomes possible to adapt the gain value of the variable-structure control part as well as the parameters characterizing the sliding surface during system operation in real time. These adaptations directly lead to a modification of the system dynamics during the transient reaching phase. This phase describes the system dynamics as long as the operating conditions do not fully comply with those system states for which the sliding condition is fulfilled. Moreover, a suitable trajectory planning procedure is presented. It allows for the specification of desired changes in the system outputs between different stationary operating points, where again the effects of limited actuator ranges and state constraints are addressed in addition with bounded uncertainty in the parameters of the nonlinear dynamic system model. Representative numerical results, based on experimental data from a test rig at the Chair of Mechatronics at the University of Rostock, are shown to conclude this contribution.

Online Industrial Mathematics

Master in Industrial mathematics (M2i): An experience with cross-institutional education in industrial mathematics

Alfredo Bermúdez, M. Elena Vázquez-Cendón, Carlos Vázquez, José Durany, Luis Bonilla and José M. Vega

Author keywords: Industrial Mathematics, Modelling, Numerical Simulation

Abstract

The Master in Industrial Mathematics (M2i) is an official degree jointly delivered by the University of Santiago de Compostela (USC), University of A Corua (UDC), University of Vigo (UVigo), Carlos III University of Madrid (UC3M) and Technical University of Madrid (UPM) since the current academic year 2013/2014. The M2i duration is 3 semesters and offers two specializations: Modelling and Numerical Simulation.

M2i degree promotes a strong dynamic relationship between the main stakeholders: students, Alumni, faculty members and professionals from industry. All information about this Spanish official Master degree can be found at the web site http://www.m2i.es/.

In this talk, on behalf of the coordinators of M2i, we highlight the main aspects of the master on the minisymposium Online Industrial Mathematics.

M2i arises from the fusion of two official degrees: the Master in Mathematical Engineering, by the universities USC, UDC and UVigo (7 editions from 2006/2007) and the Master in Industrial Mathematics, by the Carlos III University of Madrid (2 editions from 2010/20011). The main aim of the M2i is to unify subjects of high applied mathematical contents and already taught in specific engineering masters. Some ideas for this master are taken from the report by the Organization for Economic Co-operation and Development (OECD) *Global Science Forum. Report on Mathematics in Industry.*

The scientific and technological interests of the M2i mainly focus on four basic aims:

1. Expand the analytical skills and knowledge of graduate students who will be part of future research groups and professional teams.

2. Instruct the students in mathematical modelling for applications in industry.

3. Provide specific skills in relation to the design, construction and management of specific software of at least one industrial sector.

4. Introduce students to the research topics and development related to the subjects of the program.

M2i is strongly active in its relations with industry. Due to the Workshop on Industrial Problems we have signed more than 60 agreements with regional, national and international companies that collaborate with M2i. These companies present problems on which the students and teachers work in the Workshops on Industrial Problems and on Modelling. Some of these problems may become the subject of the Master s dissertation. These companies and technological centers also offer internships to students. M2i takes advantage of the IT technologies by using a modern videoconferencing system which simultaneously allows students and teachers of the different M2i sites to connect in real time. Additionally, the teaching sessions of a large part of the subjects are recorded so that the students can access the classes from home. Students have also access to professional software during the Master.

KAIST-DTU joint instruction project

Poul Hjorth

Author keywords: e-learning, collaborative mathematics, applied mathematics

Abstract

One of the elements in the strategic cooperation between Technical University of Denmark (DTU) and Korean Advanced Institute of Science and Technology (KAIST) is distance e-learning. The physical distance between the two universities is about 8.000 km, spanning 7 time zones. The cultural, and to a lesser extent educational, background of the students is different. In spring semester 2014, two courses on applied mathematics, one at each institution, briefly opened a window of distant learning, offering students a project where lectures were given by the lecturer of the other course, and project groups were formed containing students from both sites, who only met in cyberspace. This talk will report the outcome of and experience gained from that experiment.

Towards a European Net Campus for Industrial Mathematics

Matti Heilio

Author keywords: learning environment, online course, multimedia, continuing education, industrial mathematics

Abstract

The cutting edge knowledge in industrial mathematics is dispersed at small nodes of expertise. Online environments are a viable media to access this knowledge and support innovative processes, training and educational needs, to facilitate distributed consultation processes, etc.

The evolution from textbook to interactive cross media environments means a new learning paradigm. Advantages include easy access and portability, flexible updates, dynamic edition, multi/hypermedia tools from search facilities, quiz-structures to animations, interactive exercises, remote lectures and videoconference etc.

We envisage a possibility to build a European digital environment and web-portal for applied and industrial mathematics. More immediate goal is to share information and experience, describe examples of web based courses in applied mathematics and technologies for web publication of interactive documents.

Such environment would be suitable for students in applied mathematics and engineering programmes in advanced BS and MS level. It would be designed also for persons who are already in their working life and are looking for continuing education and professional development. The courses would

be based on customised content for a special applications area. Some might represent standard mathematical methods with high demand (MOOC).

A natural base for such e-learning portal would be ECMI who represents a network of European universities and collaboration with industry in mathematical technology transfer, has a mission in European knowledge sharing and an educational programme in industrial mathematics.

A first stage would be to set up a team or initiate a Special Interest Group focusing on this challenge assuming that interested partners come forward and commit themselves into exchange of ideas, experience and plans for future. This talk together with given examples of online courses is an invitation to discuss a possibility to build a European e-learning portal in applied mathematics. Let us use the time in Taormina for initiation of such a project.

Online education for mathematical modelling

Seppo Pohjolainen and Jussi Kangas

Department of Mathematics at Tampere University of Technology is coordinating a national network project on mathematical modelling. Seven Finnish universities are participating in the network project.

Author Keywords: mathematical modelling, e-learning, web-based learning.

In the project Web-based learning and teaching methods have been developed, content production for mathematical modelling has been supported and administrative measures needed to facilitate web-based learning and teaching have been put into practice. In the presentation experiences obtained from course planning, courseware production, pedagogy, didactics, technology and student feedback will be presented and analysed in detail.

Until now the language of instruction has been Finnish. In the future the courses will be given in English. This opens up a perspective for extending the national modelling education network to a European network.

Dual Delivery Courses and the Future of Online Industrial Mathematic

Leonid Kalachev and Heikki Haario

Author Keywords: online mathematics, dual-delivery courses, educational methods.

In the rapidly changing educational environment each university, researchers and educators in each scientific direction and area of knowledge should address nontrivial questions on what type of specialists will be needed by the society in the near future, how to prepare such specialists, how to continue being relevant and survive in the competition with expanding Massively Offered Online Courses (MOOCs) offered by flagship universities and with for-profit educational institutions which have already attracted substantial attention but have not yet proved or even convincingly demonstrated their effectiveness in providing the level of education required by a contemporary society and comparable to that offered by the traditional universities.

While traditional educational methods and techniques are still prevalent, to live in the age of computers and rapid communications and to pretend that they do not exist and that they do not strongly affect the delivery of educational content and overall style of contemporary education is also not acceptable. In this presentation we will share our views on the role and the place of online education in delivering content and developing necessary skills in engineering and applied mathematics disciplines. In particular, we will talk about our experience with teaching the so called dual delivery courses in applied mathematics, i.e., the courses that are being taught simultaneously in two formats, face-to-face and online. One of such unique courses com-

bining topics in Statistical, Dynamical and Computational Modeling was developed jointly by the specialists from University of Montana and from Lappeenranta University of Technology, and it has been taught for the past three years for the students at the University of Montana (face-to-face) and at University College Cork, Ireland (online).

Simulation and Optimization of water and gas networks

Adaptive Modelling, Simulation and Optimization of Water and Gas Supply Networks

Jens Lang, Pia Domschke and Oliver Kolb

Author keywords: gas and water supply networks, optimal control, numerical simulation, adaptivity, model hierarchy, adjoint-based error control, error estimators

Abstract

In this talk, I will summarize our recent activities in the field of a posteriori error estimation and model adaptation for water and gas supply networks. The concept of goal-oriented adaptivity is used to control discretization errors and a hierarchy of models during the simulation and optimization [1, 2, 3]. Beside refinement in space and variable time stepping, we want to use simplified models in regions with low activity, while sophisticated models are used in regions, where the dynamical behavior has to be resolved in detail. We introduce error estimators for the discretization and the model errors using adjoint techniques and present a strategy to automatically balance those errors with respect to a given tolerance. I will show numerical experiments for the simulation algorithm as well as the applicability in an optimization framework.

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Combination of Linear and Nonlinear Programming Techniques for Optimization Problems in Gas and Water Supply Networks

Oliver Kolb, Jens Lang, Pia Domschke, Alexander Martin, Björn Geißler and Antonio Morsi

Author keywords: gas supply networks, water supply networks, nonlinear optimization, mixed integer programming

Abstract

The operation of gas and water supply networks poses a variety of challenges. The underlying mathematical model contains a coupled system of hyperbolic PDEs, algebraic equations and ODEs. Due to the nature of the present control devices (pumps, compressor stations, valves), optimization tasks for gas and water supply networks lead to mixed integer problems. Moreover, several state constraints have to be considered.

In this talk, different approaches to tackle optimal control problems for gas and water supply networks are presented in particular a combination of mixed integer linear programming and nonlinear programming [1]. In the LP context, we apply an adaptive linearization technique. To solve the NLPs, we use derivative-based optimization techniques and a first-discretize adjoint approach [2]. Here, integer variables are given by an outer MIP solver or treated with relaxation and an adapted penalization strategy.

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High order schemes on networks of conservation laws

Raul Borsche

Author keywords: Hyperbolic, network, high order, ADER

Abstract

In this talk we present a higher order finite volume scheme for networks of hyperbolic conservation laws. Following the ADER framework, we compute the fluxes at the junction using higher order polynomials and the temporal derivatives of the coupling conditions.

These data can also be used to fill the ghost cells needed by a higher order reconstruction operator. We show that the method is exactly conservative and consistent in the case of a 1 to 1 coupling. Several numerical examples confirm the benefits of a high order coupling procedure for high order accuracy and a stable shock capturing.

We also compare the accuracy in relation to the computational costs.

From river Rhine alarm model to water supply network simulation by the method of lines

Gerd Steinebach [86]

Abstract

In this talk an overview on modelling techniques and numerical methods applied to problems in water network simulation is given. The considered applications cover river alarm systems [1], water level forecast methods [2] up to sewer and water supply networks [3].

The hyperbolic modelling equations are derived from mass and momentum conservation laws. A typical example are the well known Saint-Venant equations. For their numerical solution a conservative semi-discretisation in space by finite differences is proposed. A new well-balanced space discretisation scheme is presented which improves the local Lax-Friedrich ansatz applied so far. Higher order discretisations are achieved by WENO methods [4].

Together with appropriate boundary and coupling conditions this method of lines approach leads to an index-one DAE system. Efficient solution of the DAE system will be the topic of Tim Jaxs presentation.

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ROW methods adapted to network simulation

Tim Jax[87] and Gerd Steinebach[88]

Abstract

Simulating free-surface and pressurised flow is important to many fields of application, especially in network approaches [5]. Modelling equations to describe flow behaviour arising in these problems are often expressed by one-dimensional formulations of the hyperbolic shallow water equations. One established approach to realise their numerical computation is the method of lines based on semidiscretisation in space [4]. It leads to index-one DAE systems as algebraic constraints are required to realise coupling and boundary conditions of single reaches.

Linearly implicit ROW schemes proved to be effective to solve these DAE systems [2]. However, under certain conditions an extended partial explicit time-integration of the shallow water equations could be worthwhile to save computational effort. To restrict implicit solution by ROW schemes to stiff components while using explicit solution by RK methods for remaining terms, we present adapted AMF-IMEX schemes based on ROW method ROS34PRW [1, 3]. Applied to first test problems regarding open channel flow, their efficiency is analysed with respect to flow behaviour. Results prove to be advantageous especially concerning dynamical flow.

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Model order reduction via quadratic-linear system for nonlinear-parametric partial differential equation system

Yi Lu, Nicole Marheineke and Jan Mohring

Author Keywords:model oder reduction, quadratic-linear system, nonlinear-parametric PDE

This talk deals with model reduction for nonlinear-parametric partial differential equation system. We present an approach based on the transfer function of a quadratic-linear system for the semi-discrete nonlinear-parametric partial differential equation system. The approach will be applied to gas networks.

Modeling and optimization of gas networks

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Keywords:gas network, mixed integer programming, sequential linear programming, control theory, nonlinear problem, mathematical analysis, existence theorem

Abstract

Due to their nature, gas transmission networks occupy vast expanses of land, which, may be measured in thousands of kilometers. They are generally managed from a control center by the Technical System Manager (TSM) based on the data they receive from the different elements that form a network, namely, compression stations, pressure control valves, flow control valves, closing valves, regasification plants, international connections and underground storages.

Combining the size of the network and the number of elements which form it, managing the gas network becomes a really complex problem. Furthermore, the compression stations and regasification plants use the gas itself as an internal power source, thereby consuming their own resources. For this reason, it is necessary to pay particular attention to the way in which a network is managed.

Currently, the aim of managing a gas transportation network is to meet all consumer demands, without considering the energy cost. In other words, the aim is to guarantee the security of the supply, independently of its associated costs.

On the other hand, it is important to study the performance of the gas network in the future in order to create long-term strategic plans that optimize the existing infrastructure and reduce the investment.

In this work we present a mathematical model which reproduces the physical behavior of the gas network, including the aforementioned elements. Unlike other related works focused on the practical part, we also show a mathematical analysis to get an existence and uniqueness theorem.

The corresponding mathematical model leads to a mixed integer nonlinear optimization problem. There are a lot of nonlinear aspects, mainly due to the pressure loss constrains in the pipes and to the gas consumption and the operation range of the compressors. The model must also account for the binary decisions regarding whether or not a given valve or compressor is active.

We propose a two-stage approach to tackle this complex problem. In the first stage we apply a Sequential Lineal Programming (SLP) approach and then we employ optimization algorithms based on Control Theory. The idea of the SLP approach is to consider a relaxation of all the nonlinear functions of the problem and solve it iteratively, improving the relaxations until the algorithm finds an *optimal* suitable solution. The complexity of gas physics and engineering are reduced while taking all discrete decisions into account, and we have to solve a mixed integer linear programming at every step. Thus, the first stage provides all discrete decisions and then a continuous nonlinear optimization problem is solved in the second stage with a mathematical approach based on Control Theory. The second stage refines the solution obtained by the SLP approach, providing a solution that uses slightly more precise formulations of the physical constraints and that may be used for the study and management of the gas network. Due to the reduced complexity in each stage, both can be solved within reasonable runtimes for relatively large gas networks.

Based on the mathematical algorithms described above, we have developed a computer program, called GANESO^{TM} (GAs NEtwork Simulation and Optimization), with different modules which, among other functionalities, optimizes and simulates gas network transportation problems.

Simulation and analysis of gas networks with MYNTS

Tanja Clees, Kläre Cassirer, Bernhard Klaaßen, Igor Nikitin and Lialia Nikitina

Author Keywords: network simulation, gas transport, graph analysis, graph coarsening, metamodeling, statistical analysis.

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

In this talk, we address several issues when solving practical applications, including modeling aspects, simulation versus optimization, initialization and graph analysis, acceleration, as well as hierarchical coarsening and metamodeling for analysis purposes. We outline solution methods and discuss some novel methods, realized in MYNTS, in more detail.

Mathematical methods in medical imaging

Non-local evolutionary models and its applications to medical images

Eduardo Cuesta and Angel Durán

Author keywords: Volterra equations, Multiscale linear models, space-vale properties, Image processing

Abstract

This work analyzes non-local and linear evolutionary based models for image processing. They are multiscale linear models where the restored image evolves according to a Volterra equation. In these models the evolution of the image is controlled by a convolution kernel. Some properties of the continuous and semi-discrete cases, along with the adaptability in the selection of the kernel to the image under study, are emphasized. Some numerical experiments will illustrate the performance of these models, paying special attention to their application to filtering and contour detection in medical imaging.

Retinal vascular network in 3D from optical coherence tomography data

Pedro Serranho, Pedro Rodrigues, Pedro Guimarães and Rui Bernardes

Author Keywords: Optical coherence tomography, Image Processing, 3D, Vascular Network.

Optical Coherence Tomography (OCT) is a non-invasive imaging modality commonly used to image the human retina in vivo. OCT output is a 3D volume of the human retina, using low-coherence light to plot the different backscattering properties within the retina and showing therefore clear differences between several layers within the retina. The common use of OCT is to measure the thickness of the retina with main application to the diagnosis of macular edema.

In addition, the importance of the retina goes beyond vision diseases. In fact, the properties of the retinal vascular network have been correlated with several cardiovascular and cerebrovascular diseases. Therefore the retina can be regarded as a window to the global vascular system status. However, the mentioned correlations have been established using 2D metrics only, making use of the depth-wise projection of the retinal vascular network in color fundus photography or angiography.

Recently, in a series of works by the same authors, it was proposed the use of OCT to identify the position of the retinal vascular network, making use of the fact that OCT incident light is absorbed by blood. This creates a depth-wise shadow in the OCT signal that allows to locate the 3D position of the vessel. This has the potential to increase the correlation power to cardiovascular and cerebrovascular diseases, since the metrics information of the retinal vessels can now be obtained in 3D.

In this work we present the latest results, namely the 3D reconstruction of the vascular retinal network within the retina, making use of OCT signal alone. In this way we achieve the reconstruction of the 3D retinal vascular network by totally noninvasive means. We will focus on the mathematics of both the reconstruction and image processing tools to achieve this goal, illustrating the use of applied mathematics in this real-life applied problem. We will also show results on the partial validation of the results.

Tracking cells in 4D biomedical images

Karol Mikula

Author Keywords: image processing, numerical methods, partial differential equations, cell tracking.

Abstract

In the talk we present new method for tracking cells in 4D biomedical images (3D+time image sequences). The method is based on extraction of the cell trajectories as smooth centered paths inside 4D spatio-temporal tree structures obtained by segmentation of 4D images. In the presented approach, the 4D segmentation is obtained by creating a spatio-temporal tubes around the cell identifiers given as a result of suitable image filtering followed by a cell detection algorithm. Then a computation of constrained distance functions inside 4D segmentation is performed by solving numerically a spatially 4D eikonal equation. Since this is a large-scale computational problem in case of real 4D image data, the parallel implementation is necessary and thus developed. By a proper combination of computed distance functions we build a potential field which is backtracked in steepest descent direction in order to get the cell trajectories. Consequently, the cell lineage tree can be constructed by detecting merging trajectories when going backward in time indicating mitosis and thus a branching node of the cell lineage tree.

Our work is motivated by the recent research in biology and medicine where the reconstruction of cell population dynamics is crucial for obtaining the cell lineage trees and study of formation and evolution of morphogenetic structures. Such research is related to embryonic development of organisms

as well as to anticancer drug design.[89]

[89]This is a common work with Nadine Peyrieras and Robert Spir.

Semi-implicit finite difference schemes for nonlinear complex diffusion processes

Adérito Araújo, Sílvia Barbeiro and Pedro Serranho

Author Keywords: finite differences, complex diffusion, image denoising, stability, convergence.

Abstract

Complex diffusion is a commonly used denoising procedure in image processing. In particular, nonlinear complex diffusion proved to be a numerically well conditioned technique that is being successfully applied in medical imaging despeckling.

This talk focuses on deriving stability and convergence results for semi-implicit finite difference schemes applied to nonlinear complex diffusion equations. We present a rigorous proof for the stability and we investigate the accuracy of the numerical solution.

In image denoising, the stability proof is important for the cases where the definition of the used image is fixed. However, in the cases where it is possible to increase the definition of the image from previous acquired ones, it is also important to establish convergence results for the filtering process.

We don't restrict our analysis to the mentioned application of interest. Instead, we consider the discretization of a general nonlinear complex diffusion model, on non uniform grids.

Some numerical experiments will be shown to confirm the theoretical analysis.

Considering uncertain data in PDE based medical image processing

Tobias Preusser

Author Keywords: Image Processing, Uncertainty Quantification, Stochastic PDEs.

Abstract

Image data used in medical image processing is in general the result of a physical measurement, e.g. a computed tomography (CT) measures the X-ray absorption, ultrasound imaging measures the acoustic scattering, etc. In natural sciences it is good scientific practice to provide measurement results with error estimates, however this is typically omitted in radiological image acquisition. When such error information is available it is natural to model the pixel values of the image as random variables, i.e. pixels do not have a fixed gray or color value. Instead, pixels have a probability density distribution that contains the information about the acquisition uncertainties. We refer to these images as stochastic images and we consider them to be elements of the tensor product space between a classical image space and a random space. Applying variational methods on stochastic images leads to stochastic partial differential equations (stochastic PDEs, SPDEs), i.e. PDEs with stochastic coefficients and/or right hand side. In the talk we will discuss the notion of stochastic images and SPDE approaches to various tasks from computer vision will be discussed. The resulting models enable us to propagate uncertainty and errors in the input data to the final result of the computer vision task. In medical imaging this can allow

to make decisions in treatment and diagnoses that take into account measurement uncertainty, e.g. in the monitoring of tumor progression during chemotherapy.

Mathematical Modelling of Drug Delivery

Drug delivery in biological tissues: a semi-analytical study

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Author keywords: diffusion-reaction equations, drug delivery, mass transfer, pharmacokinetics

Abstract

Mathematical models for drug delivery are extensively used in bioengineering and provide important contributions to the medical practice, because they constitute a powerful predictive tool for a fundamental understanding of biotransport processes. For example, many studies have been carried out to investigate the release properties of a therapeutic drug from a vehicle across the skin or of an anti-restenotic agent from a drug-eluting stent.

In order to study these processes, a two-phase mathematical model describing the dynamics of a substance between two coupled media of different properties and extents is presented. The first layer is a non-erodible polymeric platform where the drug is initially contained, and the other one is the biological tissue where the drug is directed to. A system of partial differential equation describes the diffusion and the reversible binding of drug

in both layers. Additional flux continuity at the interface and an absorbing condition at the biological medium limit are imposed.

A Sturm-Liouville problem is solved and a semi-analytical solution is given in the form of an infinite series expansion. The typical drug dynamics, the concentration levels, the optimal delivery rate are shown as outcomes of simulations and discussed in some case studies. The results are used to discuss the roles of the diffusion and reaction parameters, to evaluate drug release efficacy and to assess an optimal control strategy in the rational design of advanced delivery systems.

A mathematical model for the estimation of drug binding rates in biological tissue

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Abstract

Local drug delivery is becoming an increasingly important tool to clinicians, with devices such as drug-eluting stents, therapeutic contact lenses and transdermal patches all now routinely used in practice. This is currently an area of intense research activity due to the desire to improve current local drug delivery devices and develop new devices with novel applications. However, research efforts are being hampered by an incomplete understanding of drug redistribution in biological tissue following delivery. Several models of drug binding to tissue have been proposed in the literature but the validation of these models is limited by the difficulty in experimentally determining the many parameters of the models. In particular, drug binding-on and binding-off rates as well as the density of binding sites can be extremely difficult to measure.

In this talk we present models to describe the binding of drug to com-

ponents of tissue in an in-vitro environment. The components could be, for example, non-specific general extracellular matrix binding sites or specific binding sites on the surface of cells. While the models we present are quite general, here we focus specifically on drug binding to receptors on the surface of arterial smooth muscle cells. This is of great importance in determining arterial wall drug redistribution following the insertion of a drug-eluting stent, a device which provides a local dose of drug designed to inhibit arterial smooth muscle cell proliferation.

We consider both a linear and a non-linear model of drug binding and discuss the pros and cons of each. An analytical solution is derived for the linear model. It is then shown how the non-linear model results in a Volterra integrodifferential equation which we solve numerically and also by way of perturbation techniques. By comparing the model solution with carefully controlled experiments we show how the various parameters of the system may be estimated.

Mathematical models for drug release from affinity hydrogels

Martin Meere and Tuoi Vo

Author keywords: Affinity hydrogel, Controlled drug release, Reaction diffusion equations, Drug release profile

Abstract

Hydrogels are hydrophilic cross-linked polymer networks that have found numerous applications in the biomedical sciences. Their popularity in biomedical applications is due in part to their ability to mimic some of the key features of biological tissue. However, unmodified hydrogels do not form effective reservoirs for small molecule drugs because their composition is dominated by water, and the drug molecules typically out-diffuse from the gel over a period of a few days. Affinity-based drug delivery systems have been developed to overcome this deficiency. In these systems, the hydrogel is chemically modified to enable it to bind to the active agent of interest. The binding slows the release of the drug molecules from the gel, and the release rate can be controlled by tuning the affinity of the drug molecules for the binding sites.

In this talk, mathematical models of the reaction diffusion type are considered that describe drug binding and diffusion in hydrogels. The models are simplified by considering cases where the diffusion time scales are much longer than the reaction time scales. The non-dimensional parameters governing the drug release rate are identified, and parameter regimes are found

that lead to drug release profiles that are of interest in medical applications. The theoretical results are compared with experimental release profiles.

A coupled non-Fickian model of a cardiovascular drug delivery system

Jahed Naghipoor, Josè Ferreira and Paula De Oliveira

Author Keywords: Eluting stent, Non-Fickian diffusion, Biodegradable, Viscoelasticity, Coupled model, Numerical simulation

In recent years mathematical modeling has become an effective tool in simulating drug delivery processes. In the case of drug eluting stents it leads to a deeper understanding of the drug release mechanisms in the biodegradable coating and in the vessel wall. Although the cardiovascular drug delivery depends on very complex biochemical and physiological phenomena, a simplified release model can help to adapt the delivery profile to patient needs. In this work we present a coupled model to simulate drug delivery from a stent to a vessel wall.

The coating of the stent is biodegradable and viscoelastic properties of the vessel wall are included in the model. From a theoretical viewpoint we study the stability of the continuous model and the stability of a fully discrete model. From the numerical viewpoint two particular aspects of clinical importance are addressed: the influence of the viscoelasticity of the vessel wall and the effect of permeability of the stent coating. Concerning the first aspect we show that during an initial period of time the permeation of drug in the vessel is affected by its stiffness: the total mass of drug that enters the vessel is a decreasing function of the Young modulus. Patients who need a cardiovascular stent generally have atherosclerosis and consequently stiff vessels that have high Young modulus. To prevent an inflammatory response and the smooth muscle cell growth a correct concentration of drug must penetrate the vessel from the moment when the stent is implanted. Our

findings suggest that the initial concentration of drug in the stent should be tailored to the rheological properties of the vessel walls. The second aspect we want to stress is the control of the release profile according to the permeability of the coating: release can be speed up or delayed as different polymers are used.

Optimization of Drug-Eluting Stents

Franz Bozsak, Francois Cornat, Jean-Marc Chomaz and Abdul Barakat

Author Keywords: drug-eluting stents, gradient-free optimization, drug release dynamics.

Abstract

Drug-eluting stents (DES) have a higher risk of late stent thrombosis (LST) than bare metal stents. Because drugs used in DES inhibit endothelial cell proliferation, LST is thought to be due to delayed endothelial wound healing at the site of stent implantation. The goal of the present work is to devise optimal strategies for drug release from DES that minimize the likelihood of LST while maintaining sufficiently high drug concentrations in the arterial wall to prevent restenosis.

We have developed a computational model that describes the transport within the arterial wall of drugs released by DES. The model solves the advection-diffusion-reaction equation to describe transport of the drug within the porous arterial wall and its interactions with cells. Simulations are performed for the two common DES drugs paclitaxel and sirolimus. For the optimization, we define an objective function that maximizes drug efficacy and homogeneity while minimizing drug toxicity. Optimization is accomplished using a gradient-free algorithm based on the surrogate management framework. The two variables used in the optimization are the drug release rate from the stent and the initial drug concentration loaded onto the stent.

The results demonstrate that the optimal drug delivery strategies for paclitaxel-eluting stents (P-DES) and sirolimus-eluting stents (S-DES) are

very different. For P-DES, we identified two distinct optima, both of which require considerably lower initial drug concentrations than those used today. The difference between the two optima lies in the release time; one fast (order of an hour) and one slow (order of a year). Compared to P-DES, S-DES require a much larger amount of drug to be stored in the stent polymer.

The present results offer explanations for recent trends in DES development, demonstrate the potential for large improvements in DES design, and define guidelines for implementing these improvements.

European Study Groups with Industry

Discussion Session

Charles Holland and Hilary Ockendon

Author keywords: industry, applied mathematics, future plans

Abstract

The final session in this minisymposium will be a discussion of the effectiveness of Study Groups with Industry and how the relationship between Mathematics and Industry and other applications should be carried forward into the future.

A Flying Corps of Applied Mathematicians

Poul Hjorth

Author Keywords: Applied Mathematics, University-Industry interactions, Study Groups.

The Danish Study Group activity has recently expanded into a novel flying corps type activity. This has some similarity to an "In-House" Study Group in that there is only one company or organization in focus, but the concept is smaller in scope and duration. Typically, an ad hoc team of 3-5 mathematicians assemble (in response to a problem). They then set aside 1-2 days and work on that single problem. The problems emerge through the same channels as 'normal' study group problems, but typically have more urgency and also carry a considerably higher fee. I will give examples of problems addressed in this modus operandi, and also discuss practical aspects in contrast to the ordinary Study Group activity.

Two Industry Workshops in Berlin

Andreas Muench

Author Keywords: Industry Workshop, Study Group, Process Engineering, Photovoltaics, xerographic device.

Here we report on two "Mathematics In Industry" workshops that were held in Berlin under the sponsorship of the Weierstrass Institute and the DFG Reseach Center Matheon. Both workshops followed the Study Group format but were shorter and had a more targeted scope. The first, in 2005, focused on "Process engineering of thin liquid films" and the second one, in 2008, on "Thin film photovoltaics". We will give an overview of the two workshops, the motivation behind choosing a specific focus and the experience with these two events, as well as with one of the projects on xerographic devices (laser printers) that grew out of them.

European Study Groups with Industry the portuguese experience

Adérito Araújo

Author Keywords: Study Groups with Industry, Industrial Mathematics, Success Stories.

Mathematical Study Groups with Industry were originated in Oxford in 1968 under the name of Oxford Study Groups with Industry. The concept has been adopted by other countries, and these events have become a well-established institution and the leading workshop for the interaction between mathematics and industry in Europe and in the world. But despite its success, it is not easy to introduce the concept in a country and get the workshop running in a sustainable way [1]. Major difficulties arise on both academic and industrial sides.

The first study group to be hosted in Portugal was the 60th in the European Study Groups with Industry series. It took place in Lisboa in May 2007 and counted with the collaboration of several British specialists. Since then it has been held in various universities in Portugal in a annual basis.

In this talk we will describe the portuguese experience in organising Study Groups in three perspectives: the relationship with industry; the efforts to convince the mathematical community to become active participants and the engagement of students. We will also present some problems that have been successfully solved.[90]

[90] Pedro Freitas, European Study Groups with Industry at 40 Years, SIAM News, March 21, 2009 (http://www.siam.org/news/news.php?id=1537).

Study Groups in Ireland

Stephen O'Brien, William Lee and Joanna Mason

Author Keywords: Study Group, Ireland, Industry.

Abstract

We report progress towards building efficient interactions between industry and academic mathematicians in Ireland through the mechanism of European Study Groups with Industry. This talk will give an overview of the study groups held in Ireland to date and their impact for both industrial and academic participants.

ESGI95 the first Study Group with Industry in Bulgaria

Stefka Dimova

Author Keywords: Study Groups with Industry, ESGI95, Sofia University, Bulgaria.

Abstract

The 95th European Study Group with Industry (ESGI'95) held in Sofia, Bulgaria, September 23 - 27, 2013. It was organized by the Faculty of Mathematics and Informatics, Sofia University "St. Kliment Ohridski" (FMI, SU) in cooperation with the Institute of Information and Communication Technologies, Bulgarian Academy of Sciences (IICT, BAS) and the Institute of Mathematics and Informatics, BAS (IMI, BAS). This first for Bulgaria SGI was initiated by the European Consortium for Mathematics in Industry and it was partially supported by ECMI and OCCAM.

Thirty eight participants from Bulgaria and from abroad, divided into six groups, were working on six problems raised by five Bulgarian Companies: "Compressed representation of a partially defined integer function over multiple arguments" and "Estimation of errors in text and data processing" (Adiss Lab Lts.); "Optimization of the charging process in zinc hydrometallurgy" (KCM AD); "Mini Max Wallpaper" (Mini Max); "Laboratory calibration of a MEMS accelerometer sensor" (MM Solutions AD); "Prediction of sanding in subsurface hydrocarbon reservoirs" (ppResearch Ltd.). The last two problems and the proposed solutions will be presented and discussed at the workshop.

We will share the difficulties in the organization of this first for Bulgaria event but also what we consider as a success. As a first achievement we find the increased interest of our graduate students to real problems. Sixteen of the participants at ESGI95 were students: 1 PhD, 12 Master, 3 last year Bachelor students. They proved to be sufficiently well prepared to participate successfully in the work on the problems.

We believe that the main objectives of the SGI - to identify areas for cooperation between the Bulgarian academic community and the Bulgarian industry and to create contacts between the researchers, educators, and developers that may result in future funding on a national level - were definitely achieved. We intend to make the Study Groups with Industry an every year tradition. The next one ESGI104 is already planned for September 23-27, 2014.

A Mathematical Model for Supermarket Order Picking

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Abstract

Order picking consists in the retrieving of a number of items from the storage locations to satisfy a number of independent customers' orders. It is generally recognized as one of the most significant activities in a warehouse (Koster et al, 2007). According to different authors, the order picking accounts up to 50% (Frazelle, 2001) or even 80% (Van den Berg, 1999) of the total warehouse operating costs. The critical issue in today's business environment is to simultaneously reduce the cost and increase the speed of order picking. We address the order picking process in one of the Portuguese largest companies in the grocery business. This problem was proposed at the 92^{nd} European Study Group with Industry (ESGI92).

In this setting, each operator steers the trolley on the shop floor to select items to multiple costumers. For each order, a picker may have to walk a considerable distance. The objective is to improve their grocery e-commerce and bring it up to the level of the best international practices. In particular, the company wants to improve the routing tasks in order to decrease distances. For this purpose, a mathematical model for a faster open

shop picking was developed. In this talk, we describe the problem, as well as some preliminary results and conclusions.

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Keywords open shop order picking
capacitated vehicle routing problem
integer programming

Young Researchers' Minisymposium: High Performance Computational Finance

Model Order Reduction Techniques for Basket Option Pricing

J. P. Silva[91], J. ter Maten, M. Günther, M. Ehrhardt

Abstract

The finance world although relying more and more on mathematical models, also expects them to be fast, robust and cheap. The recent revolution in Graphical Processing Units (GPU) and Field-Programmable Gate Array (FPGA) has helped to reduce time and costs but it is ultimately algorithms which prevail. In this respect, Model Order Reduction (MOR) seems to be specially suited to financial problems as it can reduce extremely computational cost [1]. We present how and when MOR can be extremely useful and how Proper Orthogonal Decomposition (POD) stands out as a robust model order reduction technique as its applications range from linear to non-linear problem [3]. We show the validity of its application to pricing of basket options, as well as to stochastic volatility models [2], through the solution of a reduced Black-Scholes PDE. Its efficiency when compared with other pricing algorithms as well as some of its limitations are discussed concisely.

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Parallel Implementation of Particle Filtering-based Maximum Likelihood Estimation of Jump-Diffusion Model

Jinzhe Yang

Author Keywords: FPGA, Parallel Computing, Distributed Computing, Particle Filter, Maximum Likelihood Estimation, Class of Jump Diffusion Models, Parameter Estimation.

Abstract

This paper presents how Field-Programmable Gate Arrays (FPGA) are used to accelerate the Particle Filters (PF) for Parameter Estimation of Financial Models. A method using particle streams, which enables efficient evaluation of constraints and weights is introduced. We provide a case study where Maximum Likelihood Estimation (MLE) of Jump-diffusion model based on PF is performed within a reasonable time. Parallel implementation of this streaming data structure is designed, and the relationship between the number of particles and the iteration steps of the optimiser would be illustrated based on speedup result. We compare our design to implementations on CPU and cloud. We show 14x speed up for the overall design and approximately 120x speedup for particle acceleration implemented purely on FPGA.

Stochastic Grid Bundling Method: Implementation on GPU

Alvaro Leitao and Cornelis W. Oosterlee[92]

Abstract

Pricing early-exercise options under multi-dimensional stochastic processes is a major challenge in the financial sector. In [2], the authors propose a practical simulation-based algorithm called Stochastic Bundling Grid Method (SGBM). SGBM is a Monte Carlo based method for pricing multi-dimensional Bermudan options. The method is based in a combination of dynamic programming, simulation, regression and bundling of paths. In the present work, the SGBM method is taken to the extreme to extend the usability of the method, for example, to Credit Value Adjustment (CVA) calculations. In that sense, the amount of bundles and the dimensionality are increased drastically. As a consequence of this, the SGBM method become much more (almost impractically) expensive. Overall, with the increment of bundles, the iterative bundling process used in the original method takes a significant amount of time. In addition, the algorithm needs a big storage because many bundles entail much more Monte Carlo simulations. In order to make the method affordable, the General-purpose computing on graphics processing units (GPGPU) is used to parallelize the algorithm. More specifically,

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the Nvidia CUDA platform [1] is the chosen tool to reach this aim, taking advantage of its last features. Two steps of parallelization are performed, one in Monte Carlo simulation and another one in bundling calculations. Furthermore, a new way to make the bundling is proposed. This technique is more efficient than iterative version and overcomes the drawbacks caused by increasing the number of bundles and the problem dimension.

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Non-hydrostatic wave propagation with depth averaged equations: models and methods

Derivation and properties of a depth-averaged Euler system

Jacques Sainte-Marie, Marie-Odile Bristeau, Anne Mangeney and Nicolas Seguin

Author Keywords: free surface flows, dispersive models, incompressible Euler system, wave propagation

Abstract

The Saint-Venant system, often referred to as the non-linear Shallow Water equations, models the dynamics of a shallow, rotating layer of a homogeneous incompressible fluid and is typically used to describe vertically averaged flows in two or three dimensional domains in terms of horizontal velocity and depth variations. This set of equations is particularly well-suited for the study and numerical simulation of a large class of geophysical phenomena such as rivers, coastal domains, oceans or even run-off or avalanches depending on relevant source terms.

The derivation of the Saint-Venant system from the Navier-Stokes equations uses the hydrostatic assumption that consists in neglecting the vertical acceleration of the fluid. This assumption is valid for a large class of geophysical flows but is restrictive in various situations where the dispersive effects (like wave propagation) cannot be neglected.

During this presentation we present an extension of the Saint-Venant system including the non-hydrostatic/dispersive terms. The derivation process and the main properties of the proposed model are given. Especially we compare the model to the so-called Green-Naghdi model and confront them to analytical solutions. A numerical scheme for the resolution of the non-hydrostatic model and based on a kinetic finite volume solver is also presented.

Advanced Numerical Simulation of Near-shore Processes by Extended Boussinesq-type Models on Unstructured Meshes

Argiris I. Delis and Maria Kazolea [93]

Mini symposium

Non-hydrostatic wave propagation with depth averaged equations: models and methods.

Abstract

Numerical simulations are essential tools for any design activity in which water waves play a significant role. Examples of such activities can be found in the field of near-shore engineering, offshore engineering, naval engineering and environmental management. Over the past 30 years Boussinesq-type models (BTMs) have enjoyed increasing favour within the coastal engineering community for such simulations. The main reasons for this are, the

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optimal blend of physical adequacy, in representing all main physical phenomena, and the relative computational ease. Under the thrust of coastal engineering needs, BTMs have been extended to cover the dynamics of the surf zone and are currently used as both research and design tools covering a wide range of phenomena from intermediate to shallow waters. However, the accurate and efficient numerical approximation of BTMs is still in the focus of on-going research and development, especially in terms of higher-order numerical schemes, the joint modelling of intrinsic and externally added wave breaking dissipation and the adaptive mathematical/numerical description of the flow.

Along these lines, the TUCWave model [1, 2], will be presented that employs a novel well-balanced higher-order finite volume (FV) scheme for approximating the BTM of Nwogu on unstructured meshes. The model equations are rewritten in the form of a system of conservation laws and the FV scheme developed is of the Godunov type. The dispersion terms in the model are discretized using consistent discretizations to the FV framework. High-order spatial accuracy is achieved through a MUSCL-type reconstruction technique and temporal through a strong stability preserving Runge-Kutta method. A novel wave breaking treatment has been incorporated in to the mode [1] and certain criteria are established to characterize breaking waves. A high performance realization of the model will be presented. The model is applied to several benchmark cases including both regular and irregular waves and computed solutions are compared to experimental data. The results indicate that the model is robust and capable of simulating wave transformations from relatively deep to shallow water.

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Numerical approximation of a new family of Green-Naghdi equations

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The propagation of surface waves on an incompressible, homogeneous, inviscid fluid is governed by the free surface Euler equations. In shallow water, a good alternative is furnished by the *fully nonlinear and weakly dispersive Boussinesq* equations, also called *Green-Naghdi* equations. These equations were first derived in [5]. It is known [1] that they approximate the full Euler equations with a good accurracy up to the breaking point. In recent years, important research efforts have provided a solid theoretical background for this class of equations. These equations have proven to adequately describe most of the water-wave phenomena taking place in the near-shore area. The question of constructing stable and accurate numerical schemes to solve these equations have received less attention. And one major drawback is the computational cost of the numerical models based on Green-Naghdi equations.

In [2] a 1D Green-Naghdi system was introduced, together with an efficient hybrid FVM-FDM numerical method. Here, we present a new and improved family of 2D systems asymptotically equivalent to the original Green-Naghdi equations, with a structure more adapted to the computation of 2D surface waves: there is no time-dependent operator to inverse,

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leading to great computational time saving. In a second time, an optimized three-parameters system is introduced, for which the dispersive properties are improved, following the spirit of [4] for the 1D case.

We investigate here the numerical approximations of this new family of models. In a first time, we propose a 2d generalization of the hybrid method of [2] on cartesian meshes. A 5^{th} order accuracy in space WENO numerical scheme is implemented, together with a a fourth-order accuracy in time SSP-RK method. The well-balancing of the global approach is reached through a *pre-balanced* formulation [3] and we enforce a maximum-principle to ensure the positivity of the water height, adapting the recent ideas of [6].

In a second time we investigate the discontinuous Galerkin discretization of the same models, to allow higher-order accuracy and more flexibility. In the same way, preservation of motionless steady states and preservation of the water height positivity are rigorously enforced.

The resulting schemes are then validated: solitary and cnoidal waves propagation and shoaling, breaking and run-up, highly nonlinear and dispersive waves propagations over submerged bars are successfully simulated. Due to the high robustness of the models, realistic overtopping applications are also investigated.

We lastly quantify the computational time improvements brought up by these new formulations, showing that they allow to reach larger scale simulations and higher order of accuracy at a cheaper computational cost than with the original ones.

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On shoaling properties of enhanced Boussinesq models

A.G. Filippini, S. Bellec, M. Colin, M. Ricchiuto

Abstract

In the study of waves propagation and transformation in near-shore zones, one has to deal with both nonlinear and dispersive effects which make the task of accurate modeling a very difficult one. An effective approach to achieve this goal is to consider two-dimensional depth averaged models. The simplest of these models, the *nonlinear shallow water equations system*, does not account for wave dispersion and higher order asymptotic approximations need to be considered. Here we focus on the so called Boussinesq-type models. These are weakly nonlinear and they are derived under the assumption that $\epsilon = O(\mu^2)$, where $\epsilon = a/h$ represents the effects of nonlinearity and $\mu = kh$ represents the dispersion (a is the wave amplitude, k the wavenumber, h the water level).

Several families of models exist which differ from the form of the dispersive terms. These are complex operators involving high order (third order) and mixed (space and time) derivatives of the free surface and averaged velocity. The design of this terms is often based on the optimization of the dispersion characteristics of the linearized version of the equations with respect to the linearized Euler equations (Airy theory, cf. Dingemans). The analysis of the properties of the linearized equations, including both phase (or group) velocity and shoaling, provides information in the range $\epsilon << 1$. However, in practice, one often observes values of ϵ which are not negligible and even of order 1.

Since the analytical investigation of the dispersion properties of the models in the nonlinear regime seems out of reach, the challenge is to evidence

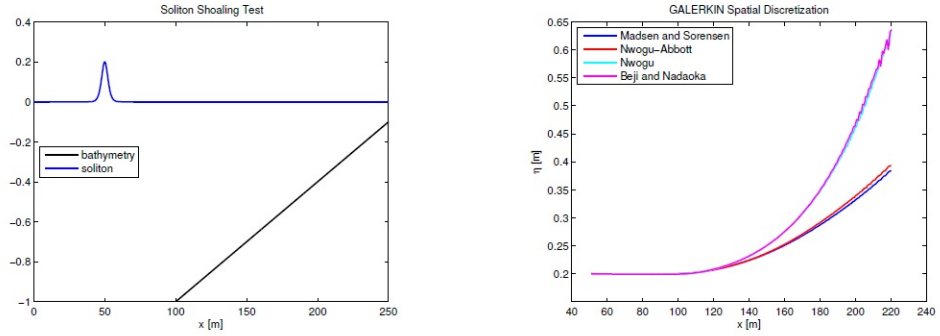

Figure 3:

some general aspects and behaviours by means of numerical tests. In this work we investigate and compare numerically the properties of two large class of models. These are all weakly nonlinear high order approximations of the Euler equations. However, they differ in the basic derivation from the fact that the asymptotic derivation is performed in terms of the free surface level (η) and the velocity (u) for one type of models, and flux (q, depth times velocity) in the others.

While in the linearized case this makes no differences at all, in the nonlinear case this provides two families of models including on one side the equations of *Peregrine [5], Beji and Nadaoka [1] and Nwogu [3]* and on the other side the models of *Abbott [2], Madsen and Sørensen [4] and Nwogu-Abbott*, which is the natural $(\eta; q)$ formulation of the equation of Nwogu. We will discuss and compare the linear properties of these models and present some numerical applications, showing that, for waves amplitude typical of the numerical benchmarks often considered in literature, their shoaling characteristics significantly differ from the ones given by the linear theory and naturally separate the two families of models. The knowledge of such properties is of paramount importance for the *a priori* choice of the proper Boussinesq- type model for the numerical simulation of the wave propagation problem in realistic environments.

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On devising Boussinesq-type equations with bounded eigenspectra: Two horizontal dimensions

Claes Eskilsson and Allan P. Engsig-Karup

Author Keywords: Nonlinear dispersive water waves, Boussinesq-type equations, Eigenvalue analysis, Spectral/hp element methods.

In enhanced Boussinesq-type equations (BE) the dispersive and nonlinear characteristics of the equations are governed by tunable parameters. In a recent paper [Eskilsson and Engsig-Karup, On devising Boussinesq-type models with bounded eigenspectra: One horizontal dimension, J. Comp. Phys. (2013)] the authors presented conditions on the free parameters under which the resulting BE will exhibit bounded eigenspectra. Using numerical computations in one horizontal dimension, with explicit time-stepping schemes, the new BE was shown to capture the physics of the wave motion as well as the standard Nwogu equation, while being much more robust and computationally efficient.

In the present paper we extend the approach to two horizontal dimensions. First we note that a two-dimensional analysis using coupled momentum equations show that the boundness of the eigenspectra extends naturally to two dimensions. However, in an earlier paper [Eskilsson and Sherwin, Spectral/hp discontinuous Galerkin methods for modelling 2D Boussinesq equations, J. Comp. Phys. (2006)] a method to rewrite the BE, using a wave continuity equation as a sub-step, was found to be computationally attractive compared to the coupled approach for spectral/hp element methods. It is illustrated that this method fails for the bounded equations and

we discuss ways to circumvent this shortcoming. Numerical computations are presented to support the analysis.

A Fast Explicit Operator Splitting Method for Modified Buckley-Leverett Equations

Chiu-Yen Kao, Alexander Kurganov, Zhuolin Qu and Ying Wang

Author Keywords: Buckley-Leverett equations, modified Buckley-Leverett equations, fast explicit operator splitting methods, central-upwind schemes, pseudospectral methods, WENO5 reconstruction.

We propose a fast explicit operator splitting method to solve the modified Buckley-Leverett equation which includes a third-order mixed derivatives term resulting from the dynamic effects in the pressure difference between the two phases. The method splits the original equation into two equations, one with a nonlinear convective term and the other one with a high-order linear terms so that appropriate numerical methods can be applied to each of the split equations: The high-order linear equation is numerically solved using a pseudospectral method, while the nonlinear convective equation is integrated using the Godunov-type central-upwind scheme. The spatial order of the central-upwind scheme depends on the order of the piecewise polynomial reconstruction: We test both the second-order minmod reconstruction and fifth-order WENO5 one to demonstrate that using higher-order spatial accuracy leads to more accurate approximation of solutions. A variety of numerical examples in both one and two space dimensions show that the solutions may have many different saturation profiles depending on the initial conditions, diffusion parameter, and the third-order mixed derivatives parameter. The results are consistent with the study of traveling wave solutions and their bifurcation diagrams.

Tailored Mathematics for the Technical Textile Industry

Setup of viscous Cosserat rod model describing electrospinning

Javier Rivero-Rodriguez, Walter Arne, Miguel Perez-Saborid, Raimund Wegener and Nicole Marheineke

Author keywords: electrospinning, Cosserat rod model, electrified jets, lateral instabilities

Abstract

Electrospinning is commonly used to produce very fine polymeric fibers. In this technique, a conducting liquid is pumped from an electrified needle into a surrounding dielectric media and the meniscus formed exhibits a conical shape, known as Taylor cone, due to the balance of electrical and surface tension forces. If the needle electrical potential is sufficiently high, the very strong electric field generated at the cone apex cannot be balanced by surface tension and a very thin jet is issued which eventually develops lateral instabilities that are responsible of additional stretching. In this work, we use a theoretical model that describes the kinematic of the midline of the jet, its radius and convective velocity from an Eulerian framework. Balance of mass, linear and angular momentum applied to a slice of the jet, as well as viscous law for stretching, bending and torsion describe the dynamics (nonlinear PDE in time and arclength of the midline). Capillary and electric forces are included in the momentum balance. If periodic orbits are explored, the time dependence of the nonlinear PDE disappears when the motion is described with respect to a frame rotating with the jet and one obtains a nonlinear BVP with its frequency as a free parameter. This

model is also suitable for describing other kinds of instabilities, such as the axisymmetric one which takes place in drop formation (dripping regime, electrospray).

Numerical solution of Cosserat rod model describing electrospinning

Walter Arne, Javier Rivero-Rodriguez, Miguel Pérez-Saborid, Nicole Marheineke and Raimund Wegener

Abstract

To simulate electrospinning asymptotic model for the dynamics of viscous jets is used. The stationary Cosserat rod is given by stiff boundary value problems. Here we present an efficient numerical approach that is based on a continuation-collocation method for the solving of the respective parameter-dependent boundary value problems. We use a Runge-Kutta method of fourth order (Lobatto IIIa formula) for the discretization and a simplified Newton method for the resulting nonlinear system. We improve the performance of the Newton method towards suitable initial guesses and global convergence by help of a continuation method. The numerical results are very convincing, they show the typical characteristic jet behavior observed in experiments.

Higher-order averaging of linear Fokker-Planck equations for fiber dynamics

Stephan Martin

Author keywords: fiber dynamics, stochastic averaging, Fokker-Planck equations, asymptotic expansion techniques

Abstract

Several models used for fiber dynamics can be rewritten as a Hamiltonian system under the influence of periodic friction and noise. We focus on a model where the Hamiltonian describes the basic motion of a single fiber, the noise summarizes stochastic influences during the lay-down process, and the friction term represents conveyor belt motion. In such a setting, one is interested in studying the energy dynamics of the system, in order to better understand the material distribution described by the model and its parameters.

In absence of friction, the energy dynamics of stochastic Hamiltonian systems can be investigated by the method of stochastic averaging. With periodic friction however, small deviations in the energy equilibrium appear which classical stochastic averaging cannot capture. Instead, we use a higher-order averaging method based on an asymptotic expansion of the associated Fokker-Planck equation around the unperturbed equilibrium, which is able to (numerically) generate averages in the subtle limit of small noise and small friction. The influence of periodic forcing hence becomes visible in second order and the new perturbed equilibria can be successfully approximated. We will present the general methodology, the numerical procedures

in use, and discuss results for fiber models.

Joint work with: A. Klar (TU Kaiserslautern), L.L. Bonilla (UC3 Madrid)

Homogenization strategies for fiber curtains/bundles in air flows

Thomas Cibis and Nicole Marheineke

Author keywords: fluid-fiber interactions, FSI, homogenization, asymptotic modeling

Abstract

In nonwoven production processes thousands of slender long fibers are swirled by an air flow and deposited onto a conveyor belt. The quality of the final fabric is thereby crucially determined by the interactions between flow and fibers. In this talk we are interested in the case of the fibers' arising in curtains or tending to bundle, then they have a strong impact on the flow and a two-way coupling of the multi-scale problem is required.

For the purpose of an efficient simulation, we investigate and compare classical homogenization techniques, a continuum approach and a superposition strategy based on an asymptotic Cosserat rod model.

Construction of artificial non-wovens

Christian H. Neβler

Abstract

We present a method for the construction of artificial non-wovens in the textile industry. The underlying model is a surrogate model for the lay-down process of non-wovens developed in earlier work. In particular, we will show a method how to construct from the many single fibres a non-woven which represents the real material. Furthermore, we will show a way how to identify contact points and how to construct a corresponding network which is the basis for artificial material tests.

Keywords

interacting particle systems, fibre dynamics, artificial materials

A moving mesh framework based on three parametrization layers for 1d PDEs

Stefan Schieβl[a96], Nicole Marheineke[a] and Raimund Wegener[b]
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Abstract

Solutions of partial differential equations (PDEs) arising in science and industrial applications often undergo large variations occurring over small parts of the domain.Resolving steep gradient sand oscillations properly is a numerical challenge. The idea of the r-renement (moving mesh) is to improve the approximation quality - while keeping the computational effort - by redistributing a xed number of grid points in areas of the domain where they are needed. In this work we develop a general moving mesh framework for 1d PDEs that is based on three parameterization layers representing referential, computational and desired parameters. Numerical results are shown for two different strategies that are applied to a ber spinning process.

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Keywords

Moving mesh, Adaptive refinement, Three parametrization layers, Fiber spinning.

Simulation of Fiber Dynamics and Fiber-Wall Contacts for Airlay Processes

Simone Gramsch, Raimund Wegener and Andre Schmeißer

Author Keywords:fiber dynamics, nonwoven production processes, fiber-fluid interaction

In an airlay process thousands of fibers are distributed by a turbulent air stream to produce a nonwoven. We present models and numerical strategies in order to simulate the dynamics of the fibers until they are laid down to a conveyor belt. In particular we focus on the effect of the turbulent air flow onto the fibers and their contact with walls. The simulation results of the lay-down can be used further, e.g., as input for interacting particle models for the fiber lay-down in nonwoven production processes.

The Airlay Process: Basic Principles and Challenges for Tomorrow

Joachim Binnig

Author Keywords: textile, simulation, fibers, CFD.

The Airlay card is one of the standard web forming machines in textile industry. It creates webs with random fiber orientation which are used for a large variety of products, including mattresses, insulation material and automotive parts. It is able to process synthetic, natural and mineral fibers; typical product area weights range from 80 to several thousand grams per square meter and throughput can be up to 1,000 kg/h per meter of working width. Despite its decade long use in textile industry, the design of machine and the operating parameters are still purely based on empirical data. This leads to the consequence that every design change and every change of fiber parameters has to be checked experimentally. For the manufacturer as well as for the operator of the machine this is a time consuming and cost intensive process. With mathematical models describing the processes inside the Airlay card, especially flow distribution and fiber lay-down, it was possible to at least partially simulate the web forming process as a function of fiber parameters and machines design as well as to identify the key influence factors on the final product quality. This would give great benefit to machine producers as well as operators and limit the cost and time effort for optimizing the Airlay card and its operating parameters.

Exploring woven structures through the geometry of Chebyshev nets

Andrew Sageman-Furnas

Author Keywords: woven structures, Chebyshev nets, discrete differential geometry, computer aided design.

Abstract

In 1878 Russian mathematicain Pafnuty Chebyshev introduced the Chebyshev net, a surface parametrization in which both partial derivatives have length one. As a material model, this corresponds to two directions along which there is little or no extension. Examples of such materials are woven structures and inextensible networks. Approximating a given shape with a woven material or inextensible network is a frequent problem both in traditional textiles (e.g. for clothing) and technical textiles (e.g. for reinforced composite materials). We investigate how far a single piece of material can be pushed to capture a shape and discuss the design implications and trade-offs which have to be made. To computationally enforce the geometric constraints we use discrete Chebyshev nets, quadrilateral meshes where all edges have the same length.

Effective Mechanical Properties of Nonwovens Produced by Airlay Processes

Christoph Strohmeyer and Günter Leugering

Author Keywords: Timoshenko, Cosserat, beams, network, homogenization, optimization.

Abstract

In modern textile industry it is of great importance to fabricate custom-tailored products which meet certain standards. To this end involved manufacturing processes have to be adjusted properly and controlled to achieve required properties. Using the example of nonwovens, the effective material behavior of stochastic fiber networks is investigated. The corresponding three-dimensional structure may be modeled as network of beams due to its geometric properties. We restrict to linear elastic geometrically exact and geometrically linear Timoshenko beams. Subsequently effective material properties can be calculated via homogenization schemes. Finally we state an optimization problem whose cost functional depends on material data of homogenized beam networks.

EU-MATHS-IN: a European Network of Mathematics for Industry and Innovation

SPRINT: Optimization of Staff Management for Desk Customer Relations Services at Hera

Matteo Pozzi, Daniele Vigo, Angelo Gordini, Claudio Caremi, Sandro Bosso, Giuseppe D'Aleo, Beatrice Beleggia, Valerio Vannini and Giulia Biancardi

Author keywords: mathematical programming, stochastic queue systems, demand forecasting, optimization

Abstract

SPRINT is a decision support system for the optimization of staff management of desk customer relations services in Hera, one of the largest Italian multi-utility company. The service is offered through a large network of 80 Customer Contact Desks (CCD) employing almost 200 persons and serving over 650.000 customers (1.1 million service requests) per year. The network is supervised by a central planning unit whereas the CCDs are controlled by local managers in charge of the operational management.

The system is based on:

- A state-of-the-art demand forecasting tool to predict the arrival of users at contact centres, based on historical data and selected service demand drivers
- A novel optimization framework based on advanced mathematical programming model approximating the nonlinear behaviour of the queue

system and consisting in three phases:

1. Determination of required staffing for each time slot (15 minutes) with an innovative adaptive staffing method explicitly tailored for this type of services,

2. Definition of the schedule that minimizes the staff required to serve the end user, through a dedicated integer linear programming model,

3. Evaluation of the average values of the service-related performance indicators by using a fast simulation engine that reproduces the working day.

The three phases are integrated into an iterative algorithm that quickly determines high quality solutions and is capable of self-adapting to the heterogeneous operational settings associated with different CCD, weekdays and demand patterns.

The developed methods experimentally proved to be superior to manual planning and to other state-of-the-art approaches. Thanks to a flexible web-based architecture, SPRINT favoured a very effective integration between central planning and the operational management of each CCD.

After more than two years' service, SPRINT has not only introduced a considerable improvement in the planning and management practices, but has also achieved a significant level-of-service improvement of desk customer services, together with relevant increase in staff productivity.

Mathematics and Patents: are these worlds compatible?

Ioannis Bozas

Author keywords: Inventions, Patents, Mathematical models, mathematical algorithms, Patent law, Patent applications

Abstract

Patent systems all over the world have consistently excluded abstract ideas from patentability. Pure mathematics and algorithms are, among other things, understood to be abstract ideas and therefore cannot be patented. However, even if no patent can be granted on a mathematical formula per se, applying said formula to solve some practical problem may result in a patentable invention. The presentation will discuss the requirements that must be met in order to get patent protection under European patent law for inventions of mathematical origin as well as differences with other patent systems. Furthermore, it will provide practical advice on how to prepare a patent application that maximizes the chances of patent prosecution with a positive outcome.

math-in | a structure to upgrade the mathematical technology transfer to industry

G. Parente and P. Quintela[97]

In this talk, it will be presented the Spanish Network for Mathematics & Industry (math-in)[98], a private non-profit organization focused on transferring mathematical technology to business and industrial sectors.

Math-in is the result of the work of a leading group of Spanish mathematicians who decided to take up the challenge of Industrial Mathematics in a innovative manner, proposing a new way to drive forward mathematical knowledge transfer, one in which the role of the researchers would be fully proactive.

One of the key differentiating features of math-in is its network structure that makes it easy for companies to access near 40 research groups, with 428 highly skilled researchers, spread throughout Spain. Research activities within the groups are aimed at specific issues of their own areas of knowledge, paying particular attention to applicability to development and innovation in companies.

According to our bylaws, math-in has the following purposes in the field of Mathematics :

- Promote and facilitate strategic relationships between researcher and industry.

[97] Spanish Network for Mathematics & Industry
[98] www.math-in.net

- Increase the presence of mathematical methods and techniques in the production sector by encouraging the participation of researchers in collaborative strategic projects with industry.
- Catalyze the valorizing of the existing knowledge through a valuable training offer addressed to the industry.
- Facilitate the internationalization of research results of researchers by fostering partnerships with other entities in other countries through participation in R&D.
- Promote and lead projects of national and international collaborative research.
- Ensure competitive advantage of researchers through the registration and exploitation of research results.
- Create a favorable environment for the creation of technology-based companies arising from research results of researchers.
- Reinforcing confidence and interest of the industry in the mathematical community.
- Strengthening the technological image of the mathematical community in Spain.

In this talk it will be presented the organization and its structure, the way to act with companies and the initiatives of MATH-IN, which allow a better coordination between research groups and thus, join forces and make the most of resources and instruments for a mutual benefit of all the members.

Efficient Image Processing Tools for Confocal Microscopy: A Case Study

Vittoria Bruni, Raino Ceccarelli, Vincenzo Ricco and Domenico Vitulano

Author Keywords:confocal microscopy, image processing, multiscale analysis

Our experience concerns some solutions to specific requirements of CrestOptics regarding confocal microscopy. The latter is a technique that has received an increasing interest in both scientific and industrial communities for specific applications such life sciences, material sciences etc. Before showing some details about our experience it is worth spending some words about it. Confocal microscopy is an optical imaging technique adopted to increase the resolution of a micrograph (i.e., a digital image acquired by a microscope to show a magnified image of an item) via point illumination and a spatial pinhole to eliminate out-of-focus light in specimens that are thicker than the focal plane. However, most of the light from sample fluorescence is lost at the pinhole. It turns out that an increase of resolution can be reached, but the price to pay is a decreased signal intensity. As just one point in the sample is illuminated at a time, imaging requires scanning over a regular raster (i.e., a rectangular pattern of parallel scanning lines) in the specimen. One of the adopted techniques for the horizontal scanning exploits a spinning disk that is composed of moving pinholes on a disk to scan spot of light. Some specific requirements from CrestOptics have been received by IAC to solve and improve particular aspects of produced microscopes. In fact, there are different aspects regarding this field that involve well-known problems in image processing like deconvolution, denoising, multiscale analysis and so on. The successful combination of some skills in mathematics and physics

along with the deep experience in this field by CrestOptics people allowed to reach some preliminary but very interesting results that can be immediately spent to realize innovative devices to launch on the market.

Setting up an industrial mathematics network and study groups in Ireland

Stephen O'Brien, William Lee and Joanna Mason

Author Keywords:study group, mathematical modelling, industry

While study groups originally started in the UK in the late 1960s and have since been exported around the world, they were only introduced to Ireland quite recently in 2008, at the university of Limerick. In this talk, I will relate some of our experiences in building up our industrial contacts and setting up the study groups from scratch and I will discuss new possibilities which may arise in the context of EU Maths-in. I will include a summary of some of our more successful study group problems.

Optimal design of Solar Power Tower systems

Emilio Carrizosa, Carmen-Ana Domínguez-Bravo, Enrique Fernández-Cara and Manuel Quero

Abstract

The design of solar power tower systems involves, among others, decisions on how many heliostats, their size, and their location in the field, as well as some technical features of the receiver (number, size, position in the tower, etc.). Under a contract financed by Abengoa Solar NT, the research team has designed a prototype implementing new algorithms to address the above mentioned issues. To do that, the different problems under consideration have been written as large-scale nonlinear nonconvex mathematical optimization problems (in some cases with integer-valued variables). Due to the large dimensionality of the problem (thousands of variables), the time-consuming evaluation of the objective function (given by a black-box procedure) and the highly nonconvex shape of the feasible region, heuristics have been developed.

As output of the project, designs with higher essiciency than those reported in the literature are being obtained, and many unexplored challenges so far have been answered as well.

Keywords: energy; solar thermal power; heliostat field layout; global optimization; heuristics

MaiMoSiNE/DOCEA Power: Assessing the quality of reduced order models of heat transfer in electronic devices

Antoine Girard[a], Pierre Lebeaut[b], Roland Hildebrand[a], Nicolas Peltier[b], Sylvian Kaiser[b]

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This talk will present the collaboration between the new structure MaiMoSiNE[99], built in the University of Grenoble to foster multidisciplinary research and interaction with industry, and DOCEA Power, which is a software vendor in the domain of semiconductors. The collaboration between MaiMoSiNE and DOCEA Power resulted from the need to improve a software tool to model and simulate heat transfer in electronic devices. DOCEA Power has developed a product to estimate the temperature of integrated circuits and printed circuit boards. The special feature of this tool is to allow the tuning of a compromise between simulation cost and accuracy.

However, users could so far only assess the quality of the results a posteriori, by comparing them to the results obtained for different sets of parameters. Works with MaiMoSiNE, made in the framework of the theory of linear dynamic systems, have allowed to find a solution so that users have a priori knowledge of the quality depending on the targeted simulation cost. The study delivered by MaiMoSiNE has helped the company to develop this new feature, which is scheduled for delivery in the next version of the prod-

[99] `http://www.maimosine.fr`

uct. The gain in productivity offered by this new feature has been validated, and the prototype is currently undergoing testing by advanced costumers.

KoMSO the German Strategic Committee for Mathematical Modeling, Simulation and Optimization

Hans Georg Bock

Author Keywords: Industrial Mathematics, German Network, KoMSO.

Abstract

The presentation will give a short review of the historical background of the German strategic committee KoMSO (komso.org) and its present and planned networking initiatives. The Committee is a strategic alliance that was founded in the wake of the Strategietag Mathematik 2020 that took place in 2010 as part of strategic dialogue activities sponsor and initiated by the German Federal Ministry of Education and Research (BMBF) since 2008. A coordination office was installed at the IWR in 2011, which is supported by the Federal Industrial Mathematics Research Funding Program "New Mathematics for Innovation in Industry and Services". The latter started in the early 90ties and has been extremely successful since. Presently, it comprises 17 collaborative research projects with partners from both industry and academic research. KoMSO is coordinated by Dr. Anja Milde and chaired jointly by the speaker, and by Professor Dr. Andreas Schuppert of Bayer AG Leverkusen. Its major activities include knitting a network of researchers and institutions from industry and academia, organization of so-called challenge workshops and modeling days on topical issues as incubators to identify and initiate collaborative research for present and future challenges for industrial mathematics, specifically in the area of mathematical modeling, analysis, simulation and optimization, and the documentation and dissemination of success stories. KoMSO is the German node within EU-MATHS-IN.

On the Italian network of Industrial Mathematics and its future developments: Sportello Matematico per l'industria italiana

Michiel Bertsch, Maurizio Ceseri, Roberto Natalini, Mario Santoro, Antonino Sgalambro and Francesco Visconti

Author Keywords: Industrial mathematics, Networking, Innovation, Technology transfer, Mathematical modeling, Simulation and optimization, Operations Research.

In this talk we present the main activities realized during the first year of the project *Sportello Matematico per lindustria italiana* (Mathematical Desk for italian industry), also referred to as SM[i]2, aiming at the development of an effective and agile network of Industrial Mathematics in Italy. Funded by the Italian Ministry of Education, University, and Research (MIUR) for a starting period of three years, SM[i]2 is being developed by the research staff of the Istituto per le Applicazioni del Calcolo Mauro Picone (IAC) at the National Research Council of Italy (CNR). The mission of SM[i]2 is to foster mathematics as a key enabling factor supporting innovation within italian companies. Thus, SM[i]2 acts as a bridge between the Italian Applied Mathematics Community and the Industry: such an ideal bridge will be progressively realized through the development of an increasing number of real collaborations between companies and research centers in industrial mathematics in Italy. The talk will briefly present the current state of the project after one year of activity. During the first year, an active scien-

tific network has been built and it is still growing: such a network involves more than twenty public and private research centers - the scientific partners of SM[i]2 - with expertise in several applications fields of industrial mathematics. The working team of SM[i]2 is composed by a number of technology translators with a scientific background in industrial mathematics; it facilitates and promotes fruitful collaborations between Italian companies and research centers selected within the above mentioned scientific network. Such collaborations are encouraged by focusing on the real needs and on the final expected benefits of the companies that request a consultancy to pursue product and process innovation. One specific target of the SM[i]2 project is to promote math-enabled innovation for an increasing number of small companies within the extremely rich network of SMEs characterizing the italian economy. Additional objectives of the project are: to stimulate the companies to hire young mathematicians; to promote the potential benefits offered by industrial mathematics by spreading the results of SM[i]2 partners success cases. Future developments of the project will be discussed as well in the talk, by presenting an analysis of the main results obtained during the first year of activities and also highlighting those promising perspectives enabled by a growing number of international collaborations.

Scheduling of Production Lines in Automotive Factories with the Modeling, Simulation and Optimization Technology

Zoltán Horváth, János Jósvai, Tamás Hajba and Sándor Kálmán

Author Keywords: scheduling of production lines, MSO technology, modeling production lines, simulation of production lines, discrete optimization, mixed integer programming, industrial application, digital factory.

Scheduling of production lines with many jobs and machines is one of the most serious tasks of an automotive factory. Several commercial software products serve decision makers on the production in their job providing them with simulation and some optimization tools. However, even the state-of-the-art software tools have limitations, in particular those for the optimization.

In order to support the scheduling decisions of engine producing segments, Audi Hungria Motor Ltd, Gyr and the Szchenyi Istvn University formed cooperations to make simulations of real production lines and their supply chains and do research for making optimization methods better. We remark that these lines are among the largest engine production lines of vehicle industry over the world.

In this talk we present our achievements in simulation, modeling and optimization for the scheduling of large scale production lines. Namely, we made contributions as follows:

- validated models and their simulations using Siemens' software Plant Simulation for real production lines and their material supply,
- optimization under Plant Simulation via built in genetic algorithms,
- set up of mathematical models of different levels (i.e. by considering more and more physical features of the lines) and implementing corresponding solvers of the type of black-box heuristics and MIP (mixed integer programming),
- construction new MIP models with efficient solvers,
- fast computational optimization the large scale problems in the mathematical models (several heuristics and MIP solvers) with interface from and to Plant Simulation,
- applications to real lines of industry.

The main conclusion is that solvers for some MIP models converge fast for several sort of large scale industrial problems and give optimum in MIP cases.

Mathematical models for wireless mesh networks

Dee Denteneer

Author Keywords: wireless mesh networks, performance modeling, statistical mechanics, Markov Renewal processes.

Wireless mesh networks are essential to realize a number of the key use case of the Internet of Things, and serve both data collection and machine to machine control. This importance is reflected in the number of products in the market that require mesh technology; within e.g. the direct experience of the speaker, there are many products for lighting control that incorporate meshing . This importance is also reflected in the number of wireless technologies that support meshing: either standards based as in Zigbee and 6LoWPAN for IEEE 802.15.4 radios and IEEE 802.11s for WiFi radios, or proprietary as CSRs recently introduced meshing technology for Bluetooth Low Energy and RF meshing for outdoor Neighborhood Area Networks. Despite their popularity, there are still many unknowns that go with the deployment of mesh networks. These unknown relate to the scalability of mesh networks, or equivalently to the performance that can be provided by a mesh network of a given size. Traditionally, the key performance metrics are throughput and fairness; however, with the use of meshing in control networks, metrics that relate to latency, synchronicity and broadcast capacity are of growing importance. The unknowns stem from the inherent broadcast nature of the wireless medium, where simultaneously transmitted messages may corrupt each other at intermittent receivers. This inherent property of wireless networks requires protocols to share the medium and these in turn invalidate traditional queueing models for the performance of data transfer. In the talk, we review the basics of the fascinating world of wireless mesh networks. We will cover products and protocols, as well as

some of the recent models developed by the speaker and co-workers to come to grip with performance. Thus, we will explore the relation of throughput in wireless networks to models from statistical mechanics. To model latency, we will resort to Markov Renewal processes and reliability theory.

PROGILE - a DS8000 storage manufacturing optimization tool at IBM DSS, Hungary

Alpar Juttner

Author Keywords: manufacturing optimization, scheduling, reconfiguration planning.

IBM DSS Hungary is the single source location of the DS8000, IBM's flagship storage systems. In order to cope with its exceptional configurability and special customer requests, IBM implements a build-to-order manufacturing scheme. The high reliability requirements necessitates an extensive - therefore time and resource consuming - testing process.

This, combined with a unique demand profile and the ubiquitous need for lowering manufacturing costs leads to a complex manufacturing process, the execution of which includes order fulfillment scheduling, order-to-parts assignment, pre-build and reconfiguration planning, based on supply availability, manufacturing capacities, existing and predicted future customer orders. This complexity naturally calls for a computer based decision support system.

As an answer to this challenge, the presentation introduces the PROGILE decision support system, developed cooperatively by IBM DSS Hungary, University of Technology and Etvs University, Budapest. It consists of prediction, optimization modules for supporting adaptive decision making at all major steps of the production process. In addition its simulation and visualization modules allows detailed what-if analysis.

AMIES : the French national network to promote interactions between mathematicians and industry

Georges-Henri Cottet

Author Keywords: mathematics, industry, SMEs.

We will present the context in which AMIES was created in 2011. We will next give an overview of the different programs proposed by AMIES, both in research and education. We will show the first results that have been obtained after 2 years. We will also discuss how we see the future of this instrument in France and how it can evolve in a European context.

MALDI Imaging: Sparsity concepts for analyzing and visualizing metabolic information

Peter Maass

Author Keywords: Sparsity, MALDI Imaging, Data imaging processing.

MALDI Imaging is a hyperspectral technology which allows to analyze proteomic/metabolic structures of tissue slices (biopsies).

This presentation starts with a short introduction for this novel imaging technology, followed by a survey on sparsity concepts in signal/image processing. We then present our approach for obtaining cluster maps with MALDI Imaging data (MSI).

The second part of this presentation is devoted to our collaboration with Bruker Daltonik, the world leading vendor of MSI hardware. We have signed an OEM (original equipment manufacturer) agreement with Bruker and since January 2013 our imaging software SCiLS Lab is sold with every MSI machine of Bruker.

We describe the process of obtaining such an agreement with a large company and highlight the particularities of involved university regulations.

An overview of HU-MATHS-IN

Zoltán Horváth

Author Keywords: industrial mathematics, applied mathematics, operations research.

The Hungarian national network of EU-MATHS-IN has been established in December 2013 to assemble the research groups working in the field of industrial mathematics in Hungary. Although these groups implemented several remarkable projects with industry and researchers working on the field of operations research formed a society from two decades, an overall national forum of industrial mathematics did not exist before. Due to the EU-MATHS-IN initiative the research groups of the country including all major institutes and universities formed the HU-MATHS-IN network.

In this talk first we flash some major achivements of the Hungarian groups from the preceding decades, including

- open loop control method for water level regulation of Balaton, the biggest lake in Central Europe,
- a model for optimal daily scheduling of the electricity production in Hungary which fulfils the technological restrictions of operating the power stations and that of the power transmitting lines,
- local daily agro-meteorological models with validated results for dry and wet periods,
- decision models for the planning of highway pavement improvements in Hungary.

Then we present some recent success stories of the HU-MATHS-IN members. These projects cover applications on a broad range of industry, among

others

- compressed representation of physiological signals for Telenor Hungary,
- optimal long term locomotive assignment planning for the Hungarian Railways,
- workforce management and operator scheduling of call centers at Telenor and ELMÜ,
- surveillance car route optimization with BKK (the public transport company of Budapest),
- build-to-order manufacturing optimization at IBM-DSS, Vác,
- simulation and optimization of production lines for Audi Hungária Motors,
- large scale risk analysis in banking for OTP Bank,
- quantified risk estimation and a simulation tool for Aegon Hungary,
- modelling the strategies for age specific vaccination scheduling during in uenza pandemic outbreaks,
- optimal time-based ticket pricing policy of urban public transportation for City of Szeged,
- Smarter Transport related activities with IBM,
- development and simulaton of fuel cells for MVM Hungarian Electricity Ltd.

Finally, we outline our plans, ideas and initiatives on networking, research and innovation, both at research group and HU-MATHS-IN level.

EU-MATHS-IN: an introduction

Wil Schilders

Author Keywords: industrial mathematics, innovation, European service network.

EU-MATHS-IN, the European Service Network of Mathematics for Industry and Innovation, is a new initiative to boost mathematics for industry in Europe. It strives to make the most of our combined expertise for a more efficient route to innovation.

EU-MATHS-IN aims to leverage the impact of mathematics on innovations in key technologies by enhanced communication and information exchange between and among the involved stakeholders on a European level. It shall become a dedicated one-stop shop to coordinate and facilitate the required exchanges in the field of application-driven mathematical research and its exploitation for innovations in industry, science and society. For this it shall build an e-infrastructure that provides tailored access to information and facilitates communication and exchange by player-specific sets of services. It will act as facilitator, translator, educator and link between and among the various players and their communities in Europe.

This presentation will serve as an introduction to EU-MATHS-IN, the road towards the birth of this network, and the general aims, mission and objectives.

Model order reduction within the electronics industry

Wil Schilders

Author Keywords: model order reduction, industrial mathematics, RLC systems, interconnect structures, linear MOR, non-linear MOR.

Model order reduction, that is, reducing the size of discrete models describing physical or other processes and phenomena in an automatic way, is receiving much attention in the past 20 years. Techniques for linear problems are in a mature state, even though there are still many interesting challenges to be addressed whereas for non-linear, parameterized and coupled problems, the theory is being developed continually.

The electronics industry is one of the main contributors to the advancement of model order reduction. Many examples stem from this area, and are inspirational for the further development. Reduction of large RLC systems, reduction of systems describing the behavior of interconnect structures, and many non-linear, parameterized and coupled problems.

In this presentation, we will show some of the applications of model order reduction in the electronics industry, and will also demonstrate the subtle interplay between theoretical and practical work. It is a very nice example of cross-fertilization taking place: theoretical results advancing the capabilities of designers, and challenging problems leading to new mathematics.

Simulation and Optimization of Solar Tower Power Plants

Simulation of Solar Power Towers: a techno-economical approach

Peter Schöttl, Raymond Branke, Thomas Fluri, Anna Heimsath, Peter Nitz [100]

Abstract

Solar power towers are complex systems that combine technologies from various domains. As their components show a strong mutual interaction, simulation and - in particular - optimization tool boxes must enable the researcher to examine the integral system.

Our team at Fraunhofer Institute for Solar Energy Systems ISE develops a framework for the evaluation of the overall system, integrating optical, thermal and economic models.

Optical simulations are done with the in-house raytracing tool Raytrace3D, which enables us to investigate different aspects of solar tower plants: heliostat and receiver geometries, blocking and shading, tracking errors and other optical errors, spillage and circumsolar radiation. Geometries for this general purpose raytracer can be created with different levels of detail, as required in the given R&D context.

For thermo-hydraulic simulations the in-house system simulation tool ColSim is used. Different receiver models can be coupled to the hydraulic

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heat transfer fluid cycle, which is embedded in the simulation of the entire power plant. Loss mechanisms are modelled on component level, considering convection, conduction and thermal radiation, as well as pressure losses. Again, different levels of detailing are available and can be used, depending on the R&D context.

Optical simulations are currently coupled with their thermal counterpart using solar flux maps. This tool chain allows performing annual simulations, parameter studies and, eventually, system and component optimizations. Implementing a technoeconomical optimization of the system (or components) including cost functions, as already done in a similar manner for other CSP technologies (e.g. parabolic trough or linear Fresnel solar fields), is ongoing work.

In this contribution, both the proprietary tool boxes including their general function, as well as their coupling, resulting in an overall simulation and eventually optimization tool will be presented and discussed.

Heliostat aim point optimization during operation of solar tower power plants

Andreas Reinholz, Peter Schwarzboezl, Nils Ahlbrink and Amadeus Rong

Author Keywords: solar tower operation, heliostat aim point, heuristic optimization, ant colony optimization, ray tracing

Abstract

Solar power tower systems use two-axis tracking mirrors to concentrate the direct solar radiation to a receiver on top of a tower. The receiver absorbs the concentrated radiation and transfers the heat to a working fluid, e.g. water/steam, molten salt or air. The radiation flux on the receiver surface is not homogenous and changes throughout the day. The performance and the operational safety of the receiver is strongly dependent on this flux distribution. A high concentration results in a high efficiency but also leads to thermal stress with the risk of material failure. Therefore, during the operation of a solar tower plant the receiver surface temperature is controlled continuously and the aim points of the heliostats are adapted accordingly.

Here, a software system for the optimization of the aim point distribution on receiver surfaces is presented. It is based on the efficient ray-tracing code STRAL and makes use of the ant colony meta-heuristic to optimize the assignment of the heliostats to a discrete number of aim points. It also includes the behavior of the receiver and takes local or global flux constraints into account. This software system is designed to precalculate the optimized aim point selection every 15-60 minutes during operation.

Multi-objective optimization of solar tower heliostat fields

Pascal Richter and Martin Frank

Author Keywords: Solar tower, Simulation, Multi-objective optimization, Genetic algorithm.

Abstract

We introduce a model to compute the annual performance of a heliostat field. We take into account topography, tracking errors, and the position and intensity of the sun. A computationally less expensive approach is introduced, which improves on the otherwise expensive pairwise comparison to calculate shading and blocking. Because the computational time is reduced significantly, the presented implementation is sufficiently fast to allow for heliostat field layout optimization within a couple of hours.

The optimization is executed via a genetic algorithm, which optimizes the heliostat positioning parameters as well as other design parameters, e.g. receiver tilt angle. A novel approach is used to reduce the search domain. Because the search domain delivers several local optima with comparable values of the objective function, the objective function is augmented. We use smoothing functionals to disperse the local optima, in order to get a unique global optimum. Different functionals are presented and their advantages and disadvantages are discussed.

This new heuristic is shown to improve the existing PS10 field. Additionally, on a hilly ground in South Africa, a field layout is optimized with additional constraints on the heliostat positions.

The Collaborative Workshop Initiative: The intersection of theoretical and experimental industrial science

Modelling transport through composite membranes: geometry effects

Maria Bruna and Guy Z. Ramon

Author Keywords: Membrane, Composite, Diffusion in porous media, Homogenisation, Solute transport

Composite membranes comprised of an ultra-thin coating film formed over a porous support membrane are the basis for state-of-the-art membranes, offering the possibility to independently optimise the support membrane and the coating film. However, there is limited information about transport through composite membrane structures and the implications for membrane performance in applications like desalination and water purification. In this talk we present a simple model for the diffusion of impurities through a composite membrane and examine how the effective trapping rate depends on basic geometric parameters. We discuss the interplay between the film thickness and the support porosity, and the effect of the pore distribution (periodic array vs. random pore distribution). We present numerical results for a large range of dimensionless parameters and compare them with the asymptotic solution.

An experimental and theoretical investigation of particle wall impacts in a T-junction

Daniele Vigolo, Ian M. Griffiths, Stefan Radl and Howard A. Stone

Author Keywords: multiphase and particle-laden flows, particle/fluid flow, pipe flow boundary layer.

Abstract

The presence of particles entrained in liquid flowing in confined geometries such as pipes and channels arises in a broad spectrum of areas including engineering and the natural and biological sciences. Understanding the particle behavior upon changes in flow direction is crucial in problems where particle inertia is important, such as the erosion process in pipe bends. The aim of our work is to understand and predict the mechanism of solid particle erosion (SPE) induced by dense particles flowing in the system, and the implication that a closed loop has on the intensity of this phenomenon. Our motivation started with the investigation of the water cooling loop of ITER, the prototype of a nuclear fusion reactor at the moment under construction in France. In this specific environment, in fact, the water is recirculated for several months prior to exchange, potentially increasing the concentration of debris contained within, hence the likelihood of SPE. An optimization of the working conditions and on the filtering sections are essential to improve the life of the piping system and, more important, the overall safety of the plant.

Here we present results on the impact of particles in a T-shaped channel in the laminar- turbulent transitional regime. The impacting event for a given system regime is described in terms of the particle Stokes number and the Reynolds number where, for the model local extensional flow, the latter also characterizes the ratio of particle size to thickness of the viscous boundary layer that forms in the region below the impingement. Experimental results for the impact are compared with the trajectories predicted by theoretical particle-tracing models for a range of configurations to determine the role of the viscous boundary layer in slowing down the particles and reducing the rate of collision with the substrate. In particular, a two-dimensional model based on a stagnation-point flow is used together with three-dimensional numerical simulations. We show how the simple two-dimensional model provides a tractable way of understanding the general collision behaviour, while more advanced three- dimensional simulations can be helpful in understanding the details of the flow. The implications of our results on the erosion process in an industrial piping system are discussed.

The Collaborative Workshop Initiative: The intersection of theoretical and experimental industrial science

Ian Griffiths

Author Keywords: Collaborative science, Experimentation, Mathematical modelling.

The Collaborative Workshop Initiative (CWI) is a new strategy for instigating collaboration between theoreticians and experimentalists to drive advances in industrial technological applications in areas where such complementary skills are essential. Currently entering its fourth year, this initiative now involves academics spanning 18 global research institutions, who meet annually in Oxford to work on new problems that demands multidisciplinary collaboration.

In this presentation we showcase some of the successes of the CWI to give a flavour of the meeting remit with the aim of expanding the network. We will present an overview of success stories in a range of areas, including: - The collaboration of Oxford Mathematics with the world-leading membrane company, Pall Corporation to develop a new understanding for membrane clogging. - The dynamics of snap-buckling and its application to biomedical valves, switchable optical devices and aerospace engineering, a collaboration between Oxford Mathematics and the Soft Mechanical Structures Laboratory, Virginia Tech. - The removal of paramagnetic material from water and its application to the water-purification industry, a collaboration with Oxford Mathematics and the Laboratory of Fields, Flows, and Interfaces, Ryerson University.

The minisymposium talk will discuss the future of the CWI and how to get involved, as well as setting the scene for other talks in the session that will focus on specific successful, ongoing, and new collaborations that have developed from this initiative.

Osmosis-assisted cleaning of thin-film composite membranes: Dynamics of pulse propagation

Guy Z. Ramon, Ian Griffiths and Robert Field

Abstract

Fouling of various kinds - mineral, colloidal and bacterial, continues to plague membrane-based desalination and water treatment. Hydraulic backwashing, through simple reversal of the flow through the membranes, may not be employed for thin-film composite membranes due to mechanical failure at high back-pressures. Recent studies provide preliminary evidence that flow reversal achieved through osmosis, induced by a slug of high salinity, may offer an innovative, effective and potentially chemical-free cleaning method. When employing this method, a question of operational importance arises: what is the effective region of flow-reversal, for a given system length, slug concentration and operating conditions? Here, we model the dilution of the salt slug in the spirit of classical Taylor dispersion, in an attempt to gain insight into the process dynamics.

Drying and Dispersion on Microstructures

Hein Verputten, Rick Driessen, Manas Mandalahalli and Peichun Amy Tsai [101]

Abstract

Surface modifications by chemical and physicalmeans have been recently employed to enhance hydrodynamic transport [1]. For instance, hydrodynamic slippage can be achieved by using hydrophobic microstructures, whereby an average slip velocity is present at the boundary [2]. Beyond the hydrodynamical transport, here, we present the influences of chemical wettability and physical structures on two other transport scenarios, namely drying a droplet with miniature suspensions and particle dispersion over microstructures [3]. For the former, our experimental results reveal an important role of surface wettability in the arrangement of microparticles on microstructures via evaporation of a water droplet containing small suspensions. The normal *coffee-ring* aggregation of particles close to the contact line can be altered by a chemical surface modification via a capillarity effect. For the latter, we theoretically study the dispersion of particles over hydrophobic microstructures, with a slip flow [46]. The effective diffusivity due to advection over the slippery surface depends on the slip length. These results provide practical implications for controlling particle deposition and dispersion using microstructured surfaces, useful for biological applications and membrane technology.

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Mathematical and numerical modeling of the cardiovascular system

Computational simulation of heart function with an orthotropic active strain model of electromechanics

Toni Lassila, Simone Rossi, Ricardo Ruiz-Baier and Alfio Quarteroni

Author keywords: multiphysics models, heart modelling, cardiac electromechanics,

Abstract

Fully integrated models of total heart function including the fluid dynamics inside the ventricle are on the horizon as computational algorithms become more efficient, allowing more comprehensive simulations of cardiovascular pathologies. Due to the multiscale and multiphysics nature of heart activity, a careful consideration between different algorithmic choices (monolithic vs. segregated, tightly vs. loosely coupled, explicit vs. implicit) has to be made in order to obtain the best compromise between stability and scalability. Our aim is to construct a baseline multiphysics integrated heart model that can be used to study the interaction between four basic fields related to the heart function: the cell-level electrophysiology, the subcellular activation mechanisms, the elastic deformation of the tissue, and (optionally) the ventricular fluid mechanics.

To model the electromechanical muscle contraction we use a stretch-dependent activation model based on thermodynamically consistent transversely anisotropic active strain model that is able to capture correctly the transmural thickening of the tissue. The passive mechanics model is adapted

from the seminal work of Holzapfel and Ogden and includes both fiber and sheet directional orthotropy. For the ventricular fluid-solid coupling we opt for a monolithic approach as it provides in our experience the best stability and computational efficiency for large displacement fluid-structure interaction problems. Additional ongoing work is related to the modelling of heart valves and their effect on ventricular fluid dynamics, in order to study e.g. the effect of valve pathologies on the mechanical work performed by the ventricles.

A computational model for total heart function has been implemented in the open-source finite element library LifeV (`http://www.lifev.org`) and recently released to the public. It is based on parallel solvers for the electrophysiology, solid mechanics and fluid mechanics subproblems. Mesh partitioning is performed with ParMETIS, and the linear problems are solution strategy based on multigrid or algebraic additive Schwarz preconditioners implemented within the Trilinos

Spectral Deferred Correction Methods for Adaptive Electro-Mechanical Coupling in Cardiac Simulation

Martin Weiser and Simone Scacchi

Author keywords: spectral deferred correction, monodomain equations, electro-mechanical coupling, adaptivity

Abstract

The Monodomain reaction-diffusion system describing the spread of the electrical impulse in the cardiac tissue exhibits features of very different spatial and temporal scales. Therefore, spatial and temporal adaptivity is a promising approach to reduce the computational complexity. However, spatial adaptivity by local mesh refinement incurs a substantial overhead for error estimation, grid manipulation, and reassembly of mass and stiffness matrices, which reduces the performance gain.

In this talk, we investigate the use of spectral deferred correction (SDC) methods for time stepping and their interplay with spatial and temporal adaptivity. SDC methods are simple iterative methods for solving collocation systems. Their flexibility allows to combine them in various ways with spatio-temporal adaptivity. We explore the use of many-stage schemes for amortizing adaptivity overhead over longer time steps, interleaving mesh refinement with SDC iterations for improved convergence, and local time stepping.

Coupling the Monodomain model for the electrical excitation with the quasi-static finite elasticity system modeling the mechanical contraction incurs another set of spatial and temporal scales. We explore the use of SDC methods for strong coupling including mechano-electrical feedback and their potential for multi-rate integration.

The properties of the resulting methods in terms of accuracy and computational complexity are discussed in detail at some numerical examples, including simple depolarization front propagation and spiral waves

Advances in the mathematical theory of the finite element immersed boundary method

Daniele Boffi, Nicola Cavallini and Lucia Gastaldi[102]

Abstract

The Immersed Boundary Method (IBM) is an effective mathematical model and approximation scheme for the discretization of biological systems which involve the interaction of fluids and solids. The Finite Element IBM (FE-IBM) proved to be competitive with respect to the original IBM (based on finite differences and on a suitable approximation of a Dirac delta function) in several aspects: in particular, the position of the solid can be dealt with in a natural way by taking advantage of the underlying variational formulation (thus avoiding the use of the delta function); moreover, the use of finite elements allows for sharp pressure jumps when discontinuous pressure

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schemes are adopted. Recently, a fully variational approach of the FE-IBM has been introduced, which can be shown to be unconditionally stable with respect to the time discretization. The novelty consists in the treatment of the coupling between the solid and the fluid: in the standard formulation, this is given by a differential equation stating that the velocity of the solid is equal to that of the fluid, while in the new formulation this coupling is imposed in a weak form. A rigorous mathematical analysis shows the stability of the coupling and the unconditional time stability.

Computational models of electro-mechanical interactions in the heart

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Outline

The heart is an electrically activated pump. An electrical signal propagates through the muscle tissue to trigger contraction, and the resulting movement results from interaction between the active tension developed in the muscle cells and the passive mechanical response of the tissue. This process, known as Excitation-Contraction Coupling (ECC) is supplemented by a number of feedback loops collectively referred to as mechano- electric feedback (MEF). Although the importance of MEF has yet to be accurately quantified, it is assumed to play a central role in regulation of heart contraction, by allowing the mechanical state of the tissue to directly affect electrophysiology and signal conduction.

Some of the most severe health problems in the developed world are closely linked to the mechano-electrical interactions in the heart. For instance, sudden cardiac death (SCD) and heart failure (HF) represent two of the most challenging problems for cardiologists. SCD is caused by disturbances to the electrical signal, which may have a number of causes, but one potential trigger is MEF caused by altered mechanical loading in an injured heart, for instance following a heart infarction. HF is a complex condition where the heart progressively loses its pumping ability, and is linked with structural changes on organ, tissue and cell scale, including disturbances to the ECC. Understanding the nature of ECC and MEF is essential for un-

derstanding these clinical conditions, and for improving existing diagnosis and therapy.

Computational models of cardiac function have been developed for several decades, and represent a valuable tool for understanding fundamental mechanisms of electro-mechanical coupling. However, the complexity of the processes involved is a challenge for model development, and the rapid dynamics and strong non-linearities in the models gives rise to numerical difficulties. In this presentation we will highlight two different aspects of modeling. First, we present a model for ECC, which aims to combine the common notion of *active stress* with the concept of *active strain*. The resulting constitutive model combines well established theoretical properties on a continuum level with a biophysically detailed representation of the electro-mechanical coupling.

The second part of this work focuses on MEF. Numerous MEF mechanisms have been proposed in the literature, and there are open questions regarding their relative contribution and physiological significance. We investigate these questions through a series of computer simulations on idealized and realistic geometries, and discuss the results in terms of potential clinical importance.

Impact of blood flow in ocular pathologies: can mathematical and numerical modeling help preventing blindness?

Paola Causin, Giovanna Guidoboni, Francesca Malgaroli, Daniele Prada, Riccardo Sacco and Alon Harris

Author Keywords: microcirculation, poroelasticity, tissue perfusion, medicine for the ageing society.

The human eye offers the extraordinary possibility to visualize and monitor non-invasively, in vivo, in humans, many morphological and haemodynamical features. Therefore, a large amount of data on ocular structures and macro- and micro-circulation could be obtained in a clinical setting during a patient's visit. However, the interpretation of these data remains a very challenging task, since the understanding of the physiology, bio-mechanics and fluid-dynamics of the human eye remains scarce. This unmet gap between the availability of imaging data and their elusive clinical interpretation hinders the advancement of therapeutic strategies and clinical management for many ocular diseases.

This talk will focus in particular on glaucoma - the second worldwide cause of blindness - which is clinically related to the irreversible loss of retinal ganglion cells axons. Elevated levels of intraocular pressure (IOP, fluid pressure inside the eye) are one of the major risk factors for glaucoma and, to date, reduction of IOP is the only target of available therapies. However, there is significant evidence that other factors might be involved in the

disease. In fact, many individuals with elevated IOP never develop glaucoma, while many patients continue to progress to blindness despite IOP maintained within safe levels. While elevated IOP may induce mechanical damage on the retina ganglion cells axons (mechanical hypothesis, see, e.g.,[1]), it is also reasonable to expect that the mechanical deformations of a living tissue would affect the blood flow within the tissue (haemodynamical hypothesis,[7]), and therefore the mechanical and haemodynamical viewpoints should be addressed as one coupled problem [4],[5]. Moreover, several studies indicate that a perfusion instability might significantly contribute to glaucomatous optic neuropathy [6]. The ocular blood flow is highly regulated in order to adapt to changing in metabolic needs during visual function and to compensate for varying perfusion pressures. The main cause of the perfusion instability is thought to be found in disturbed retinal vessels autoregulation in the context of a general systemic vascular dysregulation. Based on the above ideas, in this talk, we will synthetically address and discuss the results of two different mathematical models: * a first model [3], which investigates the relationship between blood flow and mechanical deformation within the tissue of the lamina cribrosa, a thin, sieve-like portion of sclera at the base of the optic nerve head, formed by a multilayered network of collagen fibers that insert into the scleral canal wall, pierced by the central retinal arteries and veins. In this model, the lamina cribrosa is described as a poroelastic material, where blood vessels are viewed as pores in a solid. Because of the interplay between mechanical and haemodynamical effects, the lamina porosity can be considered as an index of the capability of the blood to perfuse the lamina and thus to nourish ganglion cells; * a second model [2], based on an artificial anatomically-reasonable vascular network, which studies in a coupled manner the blood flow and the oxygen transport and delivery through retinal arterioles, capillaries and retinal tissue in a 3D framework. This multiscale model is used to drive the analysis of autoregulatory mechanisms in the muscle vessels and the subsequent effect of their impairment on blood flow and oxygen levels in the tissue.

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Inexact schemes for the fluid-structure interaction with application to the ascending aorta

Christian Vergara, Elena Faggiano, Maria Giuseppina Nestola and Fabio Nobile

Author Keywords: fluid-structure interaction, Newton method, Robin interface conditions, ascending aorta, stentless aortic valves.

We consider new inexact schemes for the solution of the fluid-structure interaction problem arising in haemodynamics. The fluid is modelled with the incompressible Navier-Stokes equations, whereas the structure with the non-linear exponential elastic model. These scheme are based on performing one or more approximate-Newton iterations on the monolithic FSI system, relying to partitioned algorithms where the interface position and the constitutive non -linearities are treated inexactly, allowing a big saving in the CPU time, however guaranteeing a good accuracy. We present an analysis of a model problem and applications to real cases. In particular, we consider a comparison of the wall-stresses obtained with stentless and stented aortic valves, implanted to substitute non-functioning original valves.

The Emerging Discipline of Pharmacometrics : At the Crossroad of Mathematics and Modern Pharmaceutical Sciences

Drug dose optimization in HIV treatment

Hasifa Nampala[a], Matylda Jab loblońska-Sabuka[b] and Matti Heiliö[b]
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The Human Immunodeficiency Virus (HIV) has for three decades socially and economically derailed the world and has claimed over 25 million lives Among people infected with HIV, liver disease has become the second most cause of morbidity and mortality. That is also the case for those patients who undergo the antiretoviral therapy (ART) [1]. We propose a mathematical model with consideration that HIV infects and replicates in CD4+ and hepatocytes in the liver, based on the theory that HIV reproduces effectively in these two types of cells. The model is written down as a set of ordinary differential equations representing the compartment diagram drawn in Figure 4. Moreover, ART efficacy and toxicity in form of a dose-response functions is incorporated [2]. The aim is to investigate the ability of different individual and combination therapies, to inhibit viral production in liver cells, while studying their contribution to the liver damage.

Simulation results show that various ART combinations have different levels of in uence on both therapeutic and toxic side. The findings show that with real data available for parameter estimation, this model can be used to recognize which of the currently existing treatments perform best in con- trolling the infection in the liver, as well as which one is most harmful to liver cells. This becomes a multiobjective optimization problem, with a multidimensional cost function. Our research goals aim at optimization of drug doses so that they maximize the therapeutic effects, while having minimal hepatotoxicity. The optimization problem will be solved using evolutionary computation. Markov chain Monte Carlo methods will be used to

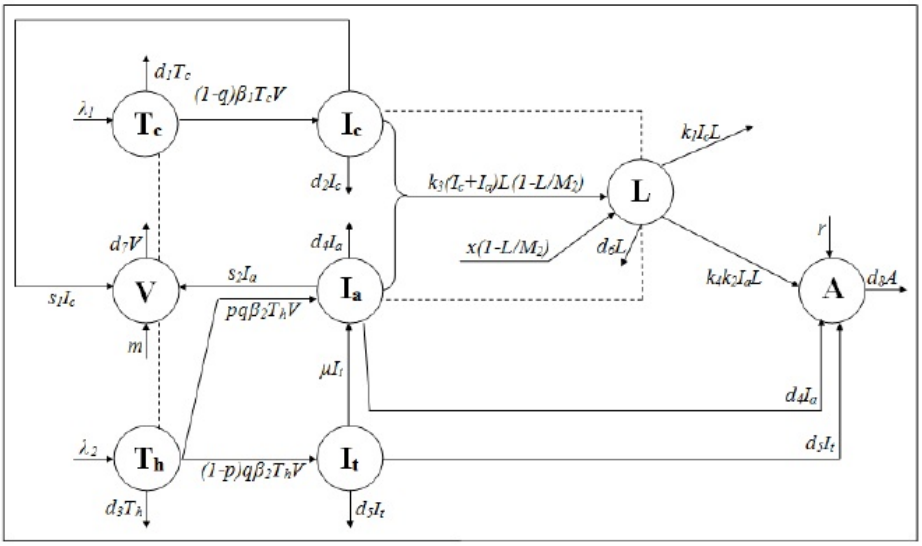

Figure 4: A compartmental diagram of the progression of HIV in the liver.

study model parameter uncertainty.

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Mathematics and CAGD: interactions and intersections

Rational Free Form Spline surfaces with Linear Transitions Maps

Hartmut Prautzsch

Author keywords: spherical Bernstein-Bezier patches, homogenous and rational splines, homogenous polarforms, Ck-manifolds, projective Staerk construction

Abstract

In Computer Aided Geometric Design (CAGD) smooth free form surfaces are typically constructed by piecewise polynomial splines which are k-times differentiable after suitable local reparametrizations. The reparametrization functions represent the coordinate changes used in differential topology to describe differential manifolds. In CAGD, they are called transition or blending functions and typically they are polynomials or splines of degree k+1 or higher. Consequently, free form surfaces with non-zero curvature are of polynomial degree 2k+2 or higher - at least in areas where the polynomial patches of the surface cannot be arranged in a regular fashion.

Employing rational polynomials, lower degree constructions are possible. As known in geometry, any manifold of arbitrary genus can be parametrized over a (so called fundamental) domain whose images under a group of motions tessellate the hyperbolic plane. The motions glue the domain to itself and represent linear rational transition maps. In 1996, Wallner used this construction of manifolds to build rational splines surfaces of arbitrary genus. In 2010, Peters and Fan derived such linear rational transition functions without using hyperbolic geometry by a purely analytic approach and

by solving the vertex enclosure problem for specific surface patch configurations. Recently in 2014, Beccari et al. promoted rational spline manifolds again over a fundamental and triangulated domain describing in more detail the Ck-joints of their rational segments.

In my talk I will present a unified, simple and elementary approach to these constructions, which allows extending Peters results to patch configurations with arbitrary knot valencies. All rational splines considered above can be represented by integral splines over affine planes which are extended to homogenous splines over the space. Conversely from any integral splines over affine planes, we can easily obtain a rational spline manifold. In particular, spherical Bernstein-Bezier surfaces introduced by Alfeld et al in 1996 can be described in this way and we can derive their common Bézier representation. For odd degree, the common and the spherical Bzier representation by Alfeld et al. have a simple geometric relationship.

Geometric clipping methods for efficient root finding

Xiaodiao Chen and Weiyin Ma [103]

Abstract

Root-finding methods have wide applications in geometry computation. Typical examples include curve/surface intersection, surface rendering, collision detection, and bisectors/medial axes computation. This talk presents an overview of geometric clipping methods for efficient root-finding of a given polynomial or an arbitrary smooth function within an interval. The main idea of the methods is to use lower order polynomial curves for bounding the roots of a higher order polynomial or an arbitrary smooth function under certain conditions. The given function is locally approximated as a lower order polynomial curve based on sample positions and relevant tangent information. Two bounding polynomials, named clipping polynomials, are further produced for bounding the roots of the original function with a substantially reduced interval. For a quadratic polynomial curve used for clipping, e.g., an optimal convergence rate of 4 can be achieved for finding a single root. In case of a cubic clipping polynomial curve, an optimal convergence rate of 6 can be achieved for finding a single root.

Key words: Root finding; tangent clipping; optimal approximation;

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convergence rate

Active contours for biomedical images based on Hermite exponential splines

C. Conti, L. Romani, V. Uhlmann and M. Unser[104]

Abstract

Cardinal Hermite exponential splines are a generalization of the classical cardinal Hermite polynomial splines with the feature of reproducing exponential polynomials. In this talk we present a new cardinal exponential B-spline basis with four elements useful for the construction of active contours for the analysis of biomedical images. Our functions provide us with a direct control over the tangents of the parameterized contour, which is absent in traditional spline-based active contours. They have been designed to perfectly reproduce elliptical and circular shapes and can approximate any closed curve up to arbitrary precision by increasing the number of anchor points. They are therefore well-suited to the segmentation of the roundish objects that are commonly encountered in the analysis of bio-images. After having established the connection to standard exponential splines, we show stability, approximation power, multiresolution properties of the new basis.

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Moreover we propose a non-stationary Hermite interpolatory subdivision scheme for refinement of vector sequences via the repeated application of level-dependent matrix subdivision operators. Finally, we illustrate the performance of our cardinal exponential B-splines constructing active contours on some examples of real biological data.

Numeric Evaluation of Geometric Continuity in CAD Systens

Tomas Sauer

Author Keywords: CAD system, Geometric continuity, Patch connection.

CAD systems usually provide information on the geometry of the underlying object in the form of patches. The smoothness of connection between adjacent patches is a fundamental quantity for many applications, in particular CAM applications like milling. The talk discusses a numerically stable way to detect and classify geometric continuity of order up to two for such adjacent patches; even if the theoretical requirements for geometric continuity are fairly well understood, the quite substantial inaccuricies and parameterization issues in real world CAD systems require mathematically sound methods in order to give a reliable evaluation of the patch connection.

Shape and Size in Biomedicine, Industry and Materials Science: an ECMI Special Interest Group

Mathematical morphology applied to the study of dual phase steel formation

Alessio A. Alessi, Vincenzo Capasso, Davide Grimaldi, Alessandra Micheletti, Daniela Morale, Junichi Nakagawa, Elena Villa[105]

Dual Phase steels (DP steels) have shown high potential for automotive and other applications, due to their remarkable property combination between high strength and good formability. The mechanical properties of the material are strictly related with the spatial distribution of the two steel phases, ferrite and martensite, and with their stochastic geometry. Unfortunately the experimental costs to obtain images of sections of steel samples are very high, thus one important industrial problem is to reduce the number of 2D sections needed to reconstruct or simulate in a realistic way the 3D geometry of the material. In this work we will present a germ-grain model which can be used to approximate the main geometric characteristics of the martensite. The parameters of the model are estimated on the basis of the morphological characteristics of the images of about 150 tomographic sections of a real sample, and confidence bands for the estimated parame-

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ters are computed. The statistical model can then be used to identify the minimum number of sections of the sample which are needed to estimate the parameters in a reliable way.

A further relevant industrial problem would be to validate a possible dynamical model on the basis of the confidence bands mentioned above, and a suitable number of numerical simulations of the mathematical model.

Mathematical Morphology of Mesoporous Alumina: Design of a 3D Random Set Model From Tem Micrographs

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Abstract

The catalytic performance and more generally the transport properties occuring in mesoporous materials are strongly influenced by the pore morphology, such as porosity, specific surface area, pore size distribution and connectivity. In the present work, we construct a 3D multiscales random model for mesoporous alumina using 2D TEM images, without prior knowledge of the nanoparticles shape and spatial aggregation. The 2D TEM images have been obtained from 300nmthick samples, much larger than the particles size. We perform a statistical analysis of the images. A bias, occuring due to space-varying sample thickness, is detected and removed using morphological operators. We identify random models from the resulting images using inverse methods. We first design a one-scale random set

model to represent the material and simulate the corresponding TEM images. A statistical comparison between the TEM images and the simulated ones shows that a second scale is needed in the random model to account for the observed spatial variations. We identify it by an optimization process, which amount to minimize a distance between the second-order statistics of the TEM images and of the simulated microstructures. The resulting probabilistic model takes into account the particles shape as well as their multiscale dispersion.

Keywords: Random media; Probabilistic microstructure models; Mesoporous materials

Stochastic modeling of engineering materials for prediction of spatial mechanical characteristics

Katharina Losch, Frank Balle, Katja Schladitz and Claudia Redenbach

Author Keywords: Al reinforced by SiC particles, SEM images, microstructure analysis, stereology, stochastic modeling.

Abstract

Reinforcing metals with ceramic particles results in changes of material properties, leading for example to increased stiffness while preserving a light weight. This is also the case for SiC reinforced aluminium alloys, making them interesting for aero-space or automotive applications.

In order to understand the material's behaviour, several deformation experiments were conducted within a scanning electron microscope (SEM). Our aim is to develop a 3D stochastic model of the material whose parameters can be estimated from 2D SEM images. Using this model, material properties can be simulated without expensive experiments improving the understanding of microstructure-property relationships. This talk reports on ongoing work in the field.

We start by segmenting the particles using an ADMM-based method. Using the segmented images, particle sizes, shapes, and their spatial distribution are analyzed. As we want to infer on 3D characteristics, stereological methods have to be applied. The analysis and model fitting are challenging since the SiC particles show complicated and possibly non-convex

shapes. Hence, standard models consisting of spherical, ellipsoidal or cylindrical grains are not suitable. Additionally, the distribution of the particles is clearly non-stationary and influenced by the manufacturing process.

Success stories from the ECMI Educational Programme

Theo-Prac Projects with Industry

Nicole Marheineke

Author keywords: modeling seminar, project in non woven production, project in robot dynamics

Abstract

Modeling seminars or modeling projects are the core in the ECMI educational program.

A special variant are Theo-Prac Projects combining theory and practice. They are embedded in a German governmental initiative to support the interaction of universities and industry and to facilitate the career entry for the students. A mathematical Theo-Prac Project has two main aims:

- mathematical modeling of an industrial project
- managing the project with respect to time, cost and man-power demands (similarly as a small company) In this talk different projects with the technical textile industry are presented.

Benefits of ECMI education in mathematical modeling: a personal reflection

Filippo Terragni

Author keywords: ECMI Educational Programme, personal experience, low dimensional modeling

Abstract

Since the very beginning of my academic education in applied mathematics, ECMI has played an important role in shaping my background and research attitude. In this talk, I will review the main stages of my personal experience within the ECMI Educational Programme, and its benefits in the development of valuable skills and knowledge in mathematical modeling.

Along all the achievements of my career, ECMI has been a major guide: since the master courses in the Universit degli Studi of Milan and the Modelling Week, passing through my MSc thesis on random shapes in microelectronics lithography (Wacker Prize 2006) jointly developed with an industry, until my PhD thesis on reduced order models in fluid dynamics, and my current position at the Universidad Carlos III of Madrid.

I will conclude my presentation by a short overview of my current research activity. In particular, I will discuss some ideas related to low dimensional modeling for the efficient construction of bifurcation diagrams in dissipative systems.

Mathematical modelling in a high school stimulated by the ECMI Educational Programme

Wojciech Okrasinski

Author Keywords: Mathematical Modelling, High School, ECMI Educational Programme.

Abstract

Since September 2009 the mathematical modelling experiment is running in a grammar-school near Wroclaw (Poland) The project entitled "Mathematical Modelling as a key to the future - the support of the mathematical education in a grammar-school" is supervised by the ECMI Teaching Center in Wroclaw University of Technology. The aim of the venture having the form of pedagogical experiment is understanding by pupils of the role of mathematics in contemporary world. Some modelling structures are copied from the ECMI educational system and applied for a high school rules. It is also remarkable that pupils with modelling activities have better final maths marks than others. Til this time the experiment is unique in Poland. But it shows that the mathematical modelling may be also introduced in high schools which are not situated in university centres.

The ingredients of an ECMI academic career

Alessandra Micheletti [106]

Abstract

I have been one of the first ECMI students at University of Milan, after the entrance of the Milan node into the ECMI Consortium. All my subsequent training and research has been strictly related with the ECMI activities, and with collaboration with Industry. I am presently associate professor of probability and mathematical statistics at University of Milan, I am chair of the ECMI Educational Committee and member of the ECMI Council. In this talk I will present how the ECMI main educational ingredients, that is training in mathematical modeling, habit in working in interdisciplinary teams and in international frameworks has improved my academic career, stimulated my research interests and inspired the training of my students in Industrial Mathematics.

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FEniCS and dolfin-adjoint: Innovative tools for automated finite element simulations

High performance computing with FEniCS

Bärbel Janssen

Author Keywords: high performance computing, turbulent flow, adaptive finite element methods.

Abstract

During the last years the simulation of large problems involving turbulent flow and deformation of solids in fluid-structure interactions has gained momentum. To be able to resolve the scales of interest we use adaptive finite element methods. Even with the use of goal oriented adaptivity the resulting discrete problems are very large.

Efficient parallelization of DOLFIN was necessary to solve this problem. This included the development of data structures and data decomposition methods for distributed unstructured tetrahedral meshes as well as efficient parallelization of local mesh refinement.

We will present the basic algorithms and applications which show the scalability and robustness of the parallelized version of DOLFIN.

Optimization of perfectly matched layers in wave propagation problems

Steven Vandekerckhove

Author Keywords: Perfectly matched layers, PDE constrained optimization, Finite element method, Adjoint problems, Wave propagation problems.

Abstract

Many wave propagation problems (acoustic, electromagnetic, elastodynamic) require the truncation of infinite domains, in order to be able to use finite meshes for numerical simulations. In the past, many custom made boundary conditions have been proposed for this purpose, however, all these appeared to be very problem specific. In 1994 Berenger proposed the use of Perfectly Matched Layers (PMLs) for solving electromagnetic problems simulated with finite difference time domain (FDTD) methods. In 1996 Chew and Jin proved that, for this case, second order polynomial attenuation functions are optimal, and suggested that these results also were to be expected for finite element methods (FEM). This work confirms this hypothesis through experiments in which the PMLs are optimized using adjoined techniques for PDE constrained optimization. Also more general attenuation functions are considered, which appear to have some benefits over the classical polynomial attenuation functions. The simulation tools FeniCS and dolfin-adjoint are indispensable for this work.

Automating the computation of Newton systems for PDE-constrained optimization

Patrick Farrell and Simon Funke

Author Keywords: adjoint, FEniCS, PDE-constrained-optimization, Newton

Abstract

Newton's method is widely considered to be the gold standard for solving optimisation problems. The key ingredients required for Newton's method are fast gradient evaluations and fast Hessian actions. In this talk, we discuss how the dolfin-adjoint software system may be used to automatically compute gradients and Hessians of functionals of PDE solvers written using FEniCS, even those of complex coupled nonlinear time-dependent equations, via the automated derivation and solution of the associated adjoint, tangent linear and second-order adjoint equations. By combining several novel techniques, these computations may become extremely efficient: with sufficient storage, both the gradient and Hessian actions may be computed in small fractions of the runtime of the forward model. (Optimal checkpointing schemes are employed when sufficient storage is not available.) These techniques rely on the automated transformation of a symbolic representation of the variational structure of the forward problem, as explicitly available in the Unified Form Language (UFL) format employed by FEniCS.

Cut finite element methods for multi-physics problems

Erik Burman, Susanne Claus, Peter Hansbo, Mats G. Larson and Andre Massing

Author Keywords: FEniCS, Cut finite element methods, Multi-physics and interface problems, computational fluid dynamics.

Abstract

Multi-domain and multi-physics problems with moving interfaces and parameter studies with changing geometric domains can be severely limited by the use of conforming meshes when complex geometries in three spatial dimensions are involved. In this talk, we focus on recent finite element methods on cut meshes (CutFEM). CutFEM technologies allow flexible representations of complex or rapidly changing geometries by decomposing the computational domain into several, possibly overlapping domains. Alternatively, complex geometries only described by some surface representation can easily be embedded into a structured background mesh.

In the first part of this talk, we briefly review how finite element schemes on cut and composite meshes can be designed by using Nitsche-type imposition of interface and boundary conditions. To make the formulations robust, optimally convergent and to avoid ill-conditioned linear algebra systems, so-called ghost-penalties are added in the vicinity of the boundary and interface.

We explain how sophisticated computational geometry methods combined with the FEniCS tool chain for automated solution of PDEs gives an efficient and easy-to-use framework for implementing schemes based on overlapping meshes and non-matching interfaces. Finally, we demonstrate how

CutFEM techniques can be employed to address various challenges from mesh generation to fluid-structure interaction problems and optimization tasks.

Semiclassical and quantum transport in semiconductors and low dimensional materials

Heat generation in the electrothermal Monte Carlo method

Wolfgang Wagner

Author keywords: Semiconductor devices, Monte Carlo simulation, Electrothermal modelling

Abstract

The kinetic equation for electron transport in semiconductors is studied. An improved version of the electrothermal Monte Carlo method is described.

This modification has better approximation properties due to reduced statistical fluctuations In addition, some new formulas for the heat generation rate are derived by analyzing the basic scattering mechanisms.

This is joint work with O. Muscato and V. Di Stefano.

Hydrodynamic transport in silicon nanowires

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Introduction

Transport phenomena in Silicon nanowire (SiNW) devices can be described using a semiclassical formulation based on the 1-D multisubband Boltzmann Transport Equation (MBTE), supposing the channel length is larger than some nanometers. The full solution of the MBTE can be obtained or by using the Monte Carlo (MC) method [**?**], [**?**], [**?**] or by using deterministic numerical solvers [**?**], [**?**] at expense of huge computational times. Another alternative is to obtain from the MBTE hydrodynamic models that are a good engineering-oriented approach. This can be achieved by taking moments of the MBTE, and by closing the obtained hierarchy of balance equations as well as modeling the production terms (i.e. the moments on the collisional operator). One way to tackle these problems is by means of the Maximum Entropy Principle (hereafter MEP) of Extended Thermodynamics [**?**], where the distribution function is assumed to be that which maximizes the entropy under the constraints of the given set of moments. In this way one obtains a representation of the distribution function valid up to the first order from Local Thermal Equilibrium (LTE), in terms of a finite number of moments.

The hydrodynamic model

By taking the moments of the MBTE, one obtains the following system of balance equations [**?**]

$$\frac{\partial \rho^\alpha}{\partial t} + \frac{\partial(\rho^\alpha V^\alpha)}{\partial z} = \rho^\alpha \sum_{\alpha'} C_\rho^{\alpha\alpha'}$$

$$\frac{\partial(\rho^\alpha V^\alpha)}{\partial t} + \frac{2}{m^*}\frac{\partial(\rho^\alpha W^\alpha)}{\partial z} + \frac{e}{m^*}\rho^\alpha \mathcal{E}_z = \rho^\alpha \sum_{\alpha'} C_V^{\alpha\alpha'}$$

$$\frac{\partial(\rho^\alpha W^\alpha)}{\partial t} + \frac{\partial(\rho^\alpha S^\alpha)}{\partial z} + \rho^\alpha e \mathcal{E}_z V^\alpha = \rho^\alpha \sum_{\alpha'} C_W^{\alpha\alpha'}$$

$$\frac{\partial(\rho^\alpha S^\alpha)}{\partial t} + \frac{6}{m^*}\frac{\partial(\rho^\alpha (W^\alpha)^2)}{\partial z} + 3\frac{e}{m^*}\rho^\alpha \mathcal{E}_z W^\alpha = \rho^\alpha \sum_{\alpha'} C_S^{\alpha\alpha'}$$

where ρ^α is the α-subband electron density in the z-direction of the wire, V^α the electron velocity, W^α the electron energy, S^α the electron energy flux, and the right-hand-side are the production terms which are known functions. We have assumed parabolic band approximation, and scattering with (bulk) optical and acoustic phonons. The above system of PDEs is of hyperbolic type, and can be numerically solved by using high-order WENO finite-difference schemes together with explicit Runge-Kutta time discretizations. Moreover, it must be coupled selfconsistently to a solution of the 2D Poisson-Schrödinger equations. Numerical simulation results for test devices will be presented at the conference.

Acknowledgment

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Modulated Bloch waves in semiconductor superlattices

M. Alvaro, L.L. Bonilla, M. Carretero
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Abstract

Bloch oscillations of the electric current through a crystal are produced by the oscillatory motion of electrons in their periodic energy bands when driven by an external electric field. They are potentially important to design infrared detectors, emitters, or lasers which can be tuned in the terahertz frequency range simply varying the applied electric field [1]. Bloch oscillations often involve multiscale problems. In this talk, we consider electrons in a superlattice made by growing alternatively layers of two different semiconductors [2]. Electron transport in the minibands of the resulting quasi-one-dimensional crystal can be described by a Boltzmann-Poisson transport model. We model electron inelastic collisions with phonons and impurities by linear relaxation to a local equilibrium that depends on the actual value of the electron density, and of its current and energy densities. In a limit of frequent almost elastic collisions, we can separate the fast time scales describing Bloch oscillations of current and energy densities from evolution at slower time scales by coarse-graining the kinetic Boltzmann-Poisson system [3]. This yields a system of partial differential equa- tions (PDEs) for the electron density, the complex envelope of the current and energy densities and the total current through the superlattice. Once these PDEs with appropriate boundary conditions are numerically solved, the electron distribution function corresponding to the fast Bloch oscillations can be reconstructed

through the singular perturbation coarse-graining procedure. In the hydrodynamic regime, at low temperature (70 K), numerical simulation of the PDEs show that terahertz Bloch oscillations of the current may coexist with several hundred times slower oscillations due to the periodic formation of electric field domains at the injecting contact of the superlattice, their motion through it and their disappearance at the collector. See the figures for current, electric field and complex envelope and for the oscillations of the total current and its Fourier transform. At room temperature, there are only Bloch oscillations with inhomogeneous stationary amplitude and electric field profiles. The Bloch oscillations disappear as the collisions become sufficiently inelastic and scattering times become sufficiently short.

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Modulated Bloch waves in semiconductor superlattices

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Abstract

Bloch oscillations of the electric current through a crystal are produced by the oscillatory motion of electrons in their periodic energy bands when driven by an external electric field. They are potentially important to design infrared detectors, emitters, or lasers which can be tuned in the terahertz frequency range simply varying the applied electric field [1]. Bloch oscillations often involve multiscale problems. In this talk, we consider electrons in a superlattice made by growing alternatively layers of two different semiconductors [2]. Electron transport in the minibands of the resulting quasi-one-dimensional crystal can be described by a Boltzmann-Poisson transport model. We model electron inelastic collisions with phonons and impurities by linear relaxation to a local equilibrium that depends on the actual value of the electron density, and of its current and energy densities. In a limit of frequent almost elastic collisions, we can separate the fast time scales describing Bloch oscillations of current and energy densities from evolution at slower time scales by coarse-graining the kinetic Boltzmann-Poisson system [3]. This yields a system of partial differential equations (PDEs) for the electron density, the complex envelope of the current and energy densities and the total current through the superlattice. Once these PDEs with appropriate boundary conditions are numerically solved, the electron distribution function corresponding to the fast Bloch oscillations can be reconstructed through the singular perturbation coarse-graining procedure. In the hydrodynamic regime, at low temperature (70 K), numerical simulation of the PDEs show that terahertz Bloch oscillations of the current may coexist with several hundred times slower oscillations due to the periodic formation of electric field domains at the injecting contact of the superlattice, their motion through it and their disappearance at the collector. See the figures for current, electric field and complex envelope and for the oscillations of the total current and its Fourier transform. At room temperature, there are only Bloch oscillations with inhomogeneous stationary amplitude and electric field profiles. The Bloch oscillations disappear as the collisions become sufficiently inelastic and scattering times become sufficiently short.

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[3] L. L. Bonilla, M. Alvaro and M. Carretero, Phys. Rev. B, **84**, 155316 (2011)

Figure 5:

Spontaneous chaos, random number generators and electron transport in multi-quantum wells at room temperature

Luis Bonilla, Mariano Alvaro and Manuel Carretero

Author keywords: spontaneous chaos at room temperature, semiconductor multi-quantum well structures, random number generators

Abstract

Physical systems that exhibit spontaneous chaos can be used as generators of truly random number sequences of interest in secure communications, encryption, improved Monte Carlo simulations, etc. Among feasible candidates, recently discovered chaotic oscillations in semiconductor multi-quantum well structures at room temperature may generate random numbers at rates as high as 100 Gb/s. We explain how electron transport in these devices produces periodic and chaotic oscillations of the current.

Characterizing spontaneous chaos in semiconductor multi-quantum wells at room temperature

Manuel Carretero, Mariano Alvaro and Luis L. Bonilla [107]

Abstract

We discuss how Poincaré maps, Fourier spectrum and multifractal dimension analysis characterize spontaneous chaos in semiconductor superlattices at room temperature.

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Derivation of a hydrodynamic model for electron transport in graphene via entropy maximization

Luigi Barletti

Author Keywords: Graphene, Hydrodynamic equations, Maximum entropy principle, Fermi-Dirac statistics

We derive semiclassical, isothermal, hydrodynamic-like equations for electrons and holes in graphene by using the maximum entropy principle. The carriers are assumed to obey the Fermi-Dirac statistics. Some general properties of such equations as well as their asymptotic forms corresponding to particular physical regimes (small and large temperature, pure state limit, diffusive limit) will be discussed.

Deterministic solutions of the transport equation for charge carrier in graphene

Armando Majorana and Vittorio Romano

Author Keywords:graphene, semiconductors, discontinuous Galerkin method, nanoribbons

Graphene is a gapless semiconductor made of a sheet composed of a single layer of carbon atoms arranged into a honeycomb hexagonal lattice. It has, as first approximation, a conical not curved band structure, so the effective mass of the electrons is zero and they exhibit a photon-like behavior. Among the graphene-based structures, the nano-ribbons are of particular importance to understand the basic transport properties of charge carriers in graphene.

A physically accurate model is given by a semiclassical transport equation whose scattering terms have been deeply analyzed in the last decade. Due to the computational difficulties, the most part of the available solutions have been obtained with direct Monte Carlo simulations.

The aim of this work is to use a numerical scheme based on discontinuous Galerkin method for finding deterministic (non stochastic) solutions of the electron Boltzmann equation in graphene. The same methods has been already successfully applied to more conventional semiconductor materials like Si and GaAs.

A n-type doping or equivalently a high value of the Fermi potential is considered. Therefore we neglect the inter band scattering but retain all the main electron-phonon scatterings.

Hydrodynamic model for charge transport in graphene

V. Dario Camiola and Vittorio Romano

Author Keywords:graphene, semiconductors, hydrodynamical models, maximum entropy principle

The aim of this paper is to formulate a hydrodynamical model for charge transport in graphene nano-ribbons based on the maximum entropy principle (hereafter MEP). The charge carriers are divided into electrons and holes in order to overcome some integrability problems related to the existence of the expectation values of interest and have a more symmetric description between the valence and the conduction band. The evolution equation for the macroscopic variables like density, energy, velocity and energy-flux are obtained by taking the moments of the transport equations. The constitutive relations needed to have a closed system of balance laws are deduced by resorting to MEP, in a way similar to the Levermore moment approach. At variance of gas-dynamics the maximization problem, MEP leads to, is proved to be globally solvable in the physically relevant region of the field variables. In the same region the evolution equation are shown to form a hyperbolic system of conservation laws.

All the main scattering mechanics are included: acoustic phonons, optical phonon and K-phonon interactions. Degeneracy is also taken into account. The model has been formulated in a planar geometry, which is the natural one for graphene nano ribbons.

Modeling and simulation of electron transport in a CNTFET

Paola Pietra and Clement Jourdana

Author Keywords: Confined nanostructures, Schroedinger equation, quantum drift diffusion model, CNT Field Effect Transistor.

Abstract

Carbon Nanotubes are complex structures that can be thought of as graphene sheets wrapped up into a cylinder. They are ultra-scaled confined structures, where the electron transport occurs in the longitudinal direction only. In nano-electronics they have great potentiality for high-speed and low-voltage switching in Field-Effect-Transistors. New models to avoid the use of the computationally demanding ab-initio computations are derived. The starting point is an effective mass model, obtained by considering the crystal lattice as periodic only in the one dimensional longitudinal direction and keeping an atomistic description of the entire cross–section. The model consists of a sequence of one dimensional device dependent Schroedinger equations, one for each energy band, in which quantities retaining the effects of the confinement and of the transversal crystal structure are inserted. A Quantum-Drift-Diffusion is then derived, following the entropy maximization approach of Degond-Mehats-Ringhofer, integrating the effective quantity of the Schroedinger approach into the definition of the entropy. In order to simulate the electron transport in a gate-all-around Field Effect Transistor, self-consistent computations include the resolution, in the whole

3D domain, of a Poisson equation describing a slowly varying macroscopic potential.

Parameterized model order reduction methods for complex multidimensional systems

Accelerating uncertainty quantification of linear simulated moving bed chromatography models by Krylov-type (parametric) model order reduction methods

Yao Yue, Suzhou Li, Lihong Feng, Andreas Seidel-Morgenstern and Peter Benner

Author Keywords: (parametric) model order reduction, Krylov methods, simulated moving bed chromatography, multi-stage system, cyclic steady state, uncertainty quantification.

Abstract

Simulated moving bed (SMB) chromatography is a class of periodically operated continuous separation processes in chemical engineering. It has been widely applied to various industrial areas ranging from petrochemicals to pharmaceuticals at all production scales. After the initial startup transient, the SMB process usually reaches a so-called cyclic steady state (CSS), which is typically used for production purpose. In robust design and optimization of SMB processes, uncertainty quantification (UQ) plays an important

role and the most popular methods are sampling-based UQ methods. To achieve high accuracy, UQ requires detailed mathematical models of SMB processes. An infinite-dimensional system of partial differential algebraic equations with periodic boundary conditions is usually used to model the hybrid behaviors of SMB. Its finite-dimensional approximation, which we use in UQ analysis, consists of a high-dimensional single-stage dynamical system that describes the continuous state evolution within each stage, along with a transition condition that represents the connection between adjacent stages. The high dimension poses a significant computational challenge to the evaluation of the CSS because computing the CSS requires either simulating the model for a large number of periods, or solving a much larger algebraic system arising from further discretizing the temporal variable. In the context of sampling-based UQ, which is a multi-query application, the computational cost becomes much higher, since the above solution procedures must be performed repeatedly.

To reduce the high computational cost, we propose to use Krylov-type (parametric) model order reduction ((P)MOR) methods, which have been successfully used in various areas such as circuit simulation, structures and vibrations, and MEMS design. In this work, we focus on SMB systems with linear adsorption isotherms.

First, we study how to extend classical Krylov-type MOR methods to reduce multi-stage SMB models. We propose a straightforward MOR method, which builds a series of ROMs, each for one stage, to deal with the multi-stage behavior of SMB processes. For more efficient UQ, we develop two strategies: the partial-update strategy and the subspace-exploiting strategy. The partial-update strategy reduces the computational cost in building reduced order models (ROMs) by updating only a small part of the bases used by MOR at each stage, while the subspace-exploiting strategy greatly reduces the number of ROMs required in sampling-based UQ analysis. Since the construction of ROMs is the computationally dominant part in sampling-based UQ analysis, the subspace-exploiting strategy can drastically reduce the computational cost.

However, Krylov-type PMOR is supposed to be more efficient for UQ analysis of SMB processes compared to Krylov-type MOR. The motivation is that, when we use MOR to accelerate sampling-based UQ analysis, we must build one new ROM for each parameter value accessed by the UQ analysis. Since sampling-based UQ analysis only accesses parameter values in a relatively small neighborhood of the nominal value, we can build a PMOR ROM that is valid for all parameter values of interest within one given stage to reduce the number of ROMs required. Therefore, when we

use Krylov-type PMOR in UQ analysis, we build a series of PMOR ROMs rather than many series of MOR ROMs. A major difficulty in using Krylov PMOR to multi-stage SMB systems is how to build PMOR ROMs so that the transition conditions with respect to all parameter values in the neighborhood are respected. In this talk, we present a sampling-based PMOR method for multi-stage linear systems, which is ideal to be combined with sampling-based UQ analysis. We also study the possibility of combining the partial-update strategy and the subspace-exploiting strategy with the proposed PMOR method.

Polynomial Chaos and Model Order Reduction for Efficient Variability Analysis

D. Spina, F. Ferranti, T. Dhæne, L. Knockaert, G. Antonini[108]

Nowadays, the analysis of the effects of geometrical or electrical parameters variability on the performance of complex high-speed systems is fundamental for a successful design. The Monte Carlo (MC) analysis is considered the standard approach for variability analysis (VA). It is easy to implement and robust, but it has a slow convergence rate, which translates in a large number of simulations. The application of the MC method for the VA of complex high-speed systems analyzed by means of electromagnetic methods (EM) [1], [2] is often unfeasible, since EM methods usually produce very large systems of equations which are expensive to solve.

Over the years, techniques [3], [4] have been proposed for the VA of systems described by large systems of equations based on combinations of a Polynomial Chaos (PC) expansion [5] and model order reduction (MOR) techniques. Despite their accuracy and efficiency with respect to the MC-based methods, these techniques can be expensive both in terms of memory and computational time, since they require the calculation of a PC-based

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model of the original large scale equations [3], [4] and of the projection matrices [4].

We propose a novel method that overcomes the previously mentioned limitations by first calculating a set of reduced order models with common order using a common compact projection matrix and then computing the PC expansion of the reduced models. We validate the accuracy and efficiency of the proposed approach with some pertinent numerical examples.

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Hi-Mod reduction driven by a POD strategy

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Author Keywords: hierarchical model reduction, proper orthogonal decomposition, data-driven methods.

Reduction of computational costs when solving complex systems of partial differential equations is progressively becoming mandatory as scientific computing is extensively used in practical applications. For this reasons, different methods for reducing the complexity and the size of the numerical problems to be solved have been investigated in the last 15 years.

In this presentation we present a method of model reduction which combines the Hierarchical Model (HiMod) reduction advocated in [1] to simplify the solution of advection-diffusion-reaction problems in pipes (or network of pipes), with the well-known Proper Orthogonal Decomposition (POD) technique [3]. We call this approach HiPOD.

HiMod is a model reduction technique to tackle phenomena characterized by a dominant dynamics, possibly featuring local relevant transverse components, like for blood flow in arteries, air in internal combustion engines, water in rivers, oil in pipes. The idea of this approach is essentially to discretize the full model via a combination of a standard 1D finite element approximation along the main stream with a modal expansion for the transverse directions. The choice of the modal basis represents a crucial issue.

POD is a well-known approach to reduce the dimensionality of a problem, by identifying its principal components in a set of snapshots computed in the off-line stage.

In the HiPOD approach the selection of the modal basis is driven via a POD procedure. In particular, we propose two different approaches, the

first one based on a standard POD projection; the second one employs a two-level POD procedure based on interpolation, similarly to what has been done in [2]. The parameter characterizing a usual POD approach assumes a different meaning in the two approaches: in the first case, it essentially collects all the problem data (problem coefficients and boundary data), while in the second case it focuses on one of the problem data. The two proposed HiPOD procedures merge the reliability typical of a HiMod approximation with the computational efficiency characterizing POD. Even though the HiPOD technique deserves to be investigated in more details, especially from a theoretical view point, the current results are very promising.

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Reduced basis method and domain decomposition for viscous flows in parametrized complex networks

Laura Iapichino, Alfio Quarteroni, Gianluigi Rozza and Stefan Volkwein

Author Keywords: reduced basis method, domain decomposition, parametrized partial differential equation, reduced order modelling, geometrical parametrization, online and offline computational decoupling, Stokes equations.

We present a reduced order method for solving to solve incompressible viscous fluid flow problems in computational domains represented by networks of repetitive geometries with heterogeneous parametrization. The main idea is to define small sets of reference domains and parameters values, then to compute once, locally and for every reference domain, some representative finite element solutions of local problems for the values of the parameter set by using parametric boundary conditions on some boundaries. The selection of the parameter set is computed through an optimal control problem. The solution of the original problem is rapidly computed, for every combination of deformed reference domains, as a Galerkin projection on the spaces defined by the local solutions previously computed. The continuity of the global solution is assured by a classical domain decomposition approach. Some numerical results show the flexibility of this approach in which accuracy and computational time may be tuned by varying the number of reduced basis or the choice of the boundary conditions at the internal interfaces of the network. By splitting the global problem into smaller local subproblems, this approach can deal with arbitrarily complex network and a

much larger global parameter space than the ones for which classical global reduced basis approach are effective.

Accelerating Optimization, Inverse Problems & Uncertainty Quantification on Complex Systems via Parameterized Model Order Reduction

Luca Daniel

Author Keywords: parameterized model order reduction, compact dynamical modeling, complex dynamical systems, design optimization, inverse problems, uncertainty quantification.

Many complex systems developed by engineers (e.g. iPads, sensor body networks, power delivery networks, magnetic resonance imaging machines) or found in nature (e.g. the human cardiovascular system, or the geophysical networks of oil/water/gas reservoirs) can be viewed as large collections of interconnected dynamical system components. The performance or characteristics of each individual component critically depend on what engineers or scientist refer to as second order effects, and can be captured only by resorting to accurate partial differential or integral equation descriptions (e.g. Poisson, Maxwell, Navier-Stokes equations etc). In addition, such components are often affected by random uncertainties in material properties and geometries. This talk will show how the state of the art in parameterized model order reduction techniques for both linear and non-linear systems can be used to enable the efficient simulation, design and optimization of entire

complex networks of interconnected dynamical systems. Examples will be presented from the electrical engineering world (e.g. integrated circuit interconnect, RF inductors, micro-electro-mechanical sensors, low noise RF amplifiers, power amplifiers, city/state wide power distribution grids) and from the biomedical world (e.g. optimization of MRI coils for reduced local heat deposition in human tissues during the next generation high resolution scans). This talk will also show how the same parameterized model order reduction techniques can also accelerate: inverse problems for oil/gas reservoir exploration; non-invasive diagnosis of diseases of the human cardiovascular system; or even most variants of the sampling based stochastic field solvers.

The use of Parameterized Cells in EDA softwares

Pascal Bolcato (Mentor Graphics Corporation)

Abstract

Parameterized Cell (PCell) is a widely used concept in the automated design of analog and custom digital electronic integrated circuits. It is a principal piece of Process Design Kit (PDK). This presentation introduces and explain this concept, including languages, interoperability and standardization concerns. It also explains the interactions between Pcells and the different parts of the design and verification flow (Layout, schematic, extraction, simulation,), for custom integrated circuit design. Then, advanced usage of Pcells are described in the context of Layout Dependent Effects (LDE), Electrical-Physical Reconciliation (EPR). And finally, the creation of macro-functions with Hierarchical PCells, is presented.

EU-MORNET: European Model Reduction Network

Wil Schilders

Author Keywords: model reduction, numerical analysis, systems and control, Krylov methods, balanced truncation, reduced basis methods.

In this presentation, we will present the newly started European network for model reduction which is a COST Action (COST is the European instrument for Cooperation in Science and Technology). This Action brings together all major groups in Europe working on a range of model reduction strategies with applications in many domains of science and technology. The increasing complexity of mathematical models used to predict real-world systems, such as climate or the human cardiovascular system, has led to a need for model reduction, which means developing systematic algorithms for replacing complex models with far simpler ones, that still accurately capture the most important aspects of the phenomena being modelled. The Action will emphasize model reduction topics in several themes: 1. design, optimization, and control theory in real-time with applications in engineering; 2. data assimilation, geometry registration, and parameter estimation with a special attention to real-time computing in biomedical engineering and computational physics; 3. real-time visualization of physics-based simulations in computer science; 4. the treatment of high-dimensional problems in state space, physical space, or parameter space; 5. the interactions between different model reduction and dimensionality reduction approaches. The focus of the Action is methodological; however, a wide range of both scientific and industrial problems of high complexity is anticipated to motivate, stimulate, and ultimately demonstrate the meaningfulness and efficiency of the Action. The main objective of the Action is to significantly bringing down computation times for realistic simulations and co-simulations of in-

dustrial, scientific, economic and societal models by developing appropriate *model reduction* methods.

Model reduction in Continuum Thermodynamics

Specific application of mathematical modelling in glass technology

Petr Schill

Author Keywords: mathematical modelling, glass flow, heat transfer, Boussinesq approximation, finite volume method, Navier-Stokes Equation

Abstract

The use of mathematical modelling in industry, particularly in glass production and processing requires specific approach due to wide complexity of the process. Modelling of glass production has to cover simultaneously several physical processes as glass batch melting, glass melt flow, heat transfer in glass melt and in glass tank, energy transfer from electric heating electrodes immersed in glass melt and from gas (or oil) burner located above the glass melt (mostly by coupling procedures), etc. Modelling of glass processing (e.g. Float glass) requires to incorporate more phenomena as visco-elastic behavior and exponential change of viscosity during glass forming.

This presentation touches just a part of all the glass-modelling problems, mainly the glass melting and flow and heat transfer in industrial glass furnaces. It was found one of the most effective numeric method in this area is finite volume method based on using finite difference procedures on non-uniform rectangular staggered grid system. There are discussed numerical aspects of the Boussinesq approximation for buoyance forces, of the Rosseland approximation for heat transfer, of the coupling of the newly melted glass with existing glass melt, and of the high aspect ratio of grid differences in vertical and horizontal directions.

It seems that most effective way of differencing of the Navier-Stokes PDE can be made by using partial integration over control volume with stabilization by exponential particular solution. This stabilization is necessary for large Pe> 2 and Re> 2. Higher precision can be achieved by transforming the difference eqs. into correction form with residuum and with new correction unknown variables. It was found that solving the flow difference eqs. is more stable and more effective by using SCGS (Symmetrical Coupled Gauss-Seidel) instead of using decoupled methods as SIMPLE or SIMPLER. The specific construction of iteration loops can support the stability and simulation rate. The above described method will be demonstrated by 3D simulation results of glass melting furnace.

Termodynamics of rate type fluid models a their applications to deformations of apshalt binders

Josef Malek

Author Keywords:rate type fluid, Maxwell fluid, Oldroyd fluid, Burgers fluid, asphalt binder, thermodynamical compatibility, viscoelastic material

For the description of complicated behavior and response of viscoelastic materials we derive a new thermodynamically compatible rate-type fluid model. We show that it is capable of capturing two non-linear relaxation responses observed in the experimental data with asphalt binder while the standard linear models are not. Furthermore, we show how to obtain the standard viscoelastic Maxwell, Oldroyd-B and Burgers' models in this thermodynamical compatible way. It is shown that the elastic part of response corresponds to that of compressible neo-Hookean solid. Finally, we use this model for the simulations in the deforming domains. Specifically, we compute two problems. In the first one we show the influence of the material parameters on the behavior of viscoelastic material. The other problem describes the rolling of incompressible ashalt binder with the real material parameters.

Mathematical modeling of float glass forming process

Vít Průša

Author Keywords: Pilkington process, multicomponent flow, diffuse interface models, glass ribbon stretching, model reduction.

Abstract

The float glass process (Pilkington process) is the standard industrial scale process for manufacturing flat glass. The initial stage of the process is the flow of the glass melt down an inclined plane (spout), and its impact on the tin bath, which makes the process an example of a multicomponent physical system. The subsequent stage of the process is the flow of a thin layer of molten glass—the ribbon—on top of the molten tin bath. This stage of the process exploits the strong temperature dependence of the viscosity of the glass melt. A careful control of the temperature in the tin bath beneath the glass melt allows one to control the thickness of the stretched glass ribbon and hence the final thickness of the manufactured flat glass. Our objective is to develop a mathematical model for the whole process that would allow one to study the impact of various operating parameters on the process, in particular on the thickness and the quality of the manufactured glass.

For the computer simulation of the initial stage of the process we use a Cahn–Hilliard–Navier–Stokes type model which conceptually belongs to the class of so-called diffuse interface models. The diffuse models treat the interface between the components as a thin layer across which the components can mix. This allows one to avoid highly specialized and difficult to implement interface tracking methods. Unfortunately, modeling the whole glass forming process using exclusively Cahn–Hilliard–Navier–Stokes type

model is unfeasible due to the size of the arising computational problem. Therefore one needs a reduced model for at least a part of the whole process that would make the problem computationally manageable. Here one can exploit the fact that the second stage of the process is dominated by the stretching of the ribbon due to the surface tension, temperature induced changes in the viscosity and the pulling of the ribbon. This type of flow calls for an application of a simplified model based on a thin film type approximation. We introduce such a model. Finally, we discuss benefits and drawbacks of Cahn–Hilliard–Navier–Stokes type model and the thin film type approximation with the vision of coupling both approaches into a unified, computationally manageable model of the whole float glass forming process.

Mathematics of fluids in motion: Analysis and/or numerics

Eduard Feireisl

Author Keywords: Navier-Stokes-Fourier system, well posedness, numerical methods in thermodynamics.

Abstract

We discuss a simple model of a compressible, viscous and heat conducting fluid. Our goal is to emphasize the synergy between analysis and numerical computations. In particular, we show how results concerning well posedness, regularity and conditional regularity of the solutions may give rise to rigorous error estimates for ceratin numerical schemes.

Selected Topics in Semi-Classical and Quantum Transport Modeling

Pseudopotential-based study of electron transport in low-dimensionality nanostructures

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Abstract

Scaling electronic devices to (and beyond) the 10 nm gate-length will likely require intrinsically two-dimensional (2D) materials. This stems from the necessity of confining electrons within the thickness required by conventional scaling laws, avoiding the intolerable gate leakage currents that result from the shift of the ground-state subband induced by quantum confinement[1].

Pseudopotentials empirical and *ab initio* are now being more commonly used to study not only the atomic and electronic structure of these 2D materials (e.g., graphene, silicene, transition-metal dichalcogenides -TMDs), but also their electronic transport properties. Here we shall give a birds-eye view of the use of density functional theory (DFT) to calibrate empirical pseudopotentials (EPs), of EPs to calculate efficiently the electronic structure of low-dimensionality systems, the most significant electronic scattering processes, and to study semiclassical electronic transport. Low-dimensionality systems considered here include thin semiconductor layers, graphene, bilayer graphene, graphene- and silicane-nanoribbons, silicon nanowires, TMDs and single-layer Sn (*stannanane*).

Regarding graphene, the high electron mobility measured in suspended

graphene sheets[2] ($\backsim$ $200,000 cm^2/Vs$) is the result of a relatively weak carrier-phonon coupling and the strong dielectric-screening property. However, in practical applications graphene is likely to be supported by an insulating substrate, top-gated, and possibly used in the form of narrow armchair-edge nanoribbons (AGNRs) in order to open a gap. We will discuss several scattering processes that may affect electron transport in these situations. First, we shall present results of the calculation of the intrinsic electron-phonon scattering rates in suspended graphene and AGNRs using empirical pseudopotentials[3] and the rigid-ion approximation[4] or DFT calculated deformation potentials[5], resulting in an electron mobility consistent with the experimental results. We shall then discuss the role of interfacial coupled substrate optical-phonon/graphene-plasmons[6] (i.e., remote phonons) in depressing the electron mobility in graphene supported by SiO_2, HfO_2, Al_2O_3, and h-BN. We shall also review the strong effect of line edge roughness (LER) on electron transport and localization in narrow AGNRs[7] resulting from the 'claromatic width dependence of the band-gap of the sp^2-coordinated AGNRs. This will lead us to consider sp^3-coordinate ribbons (silicane) and Si nanowires as possible alternative structures - less affected by LER scatterin-g of interest in nano-electronics application.

Finally, we shall discuss the effect of high-κ gate dielectrics to boost the mobility of MoS_2 single layers, DFT calculations of the properties of halogen-terminated stannanane as a 2D topological insulator, and the effect of ideal metallic gates in suppressing the normal-superfluid transition-temperature in graphene bilayers.

This work has been performed in collaboration with S. J. Aboud (Stanford), W. G. Vandenberghe, A. Suarez-Negreira, Z.-Y. Ong, J. Kim, S. Narayanan, Bo Fu, and C. Sachs (UT-Dallas) and has been supported by NRI/SWAN2.0

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Simulation of Oxide Reliability of nanoscaled MOSFETs using Drift-Diffusion, Monte Carlo and Full-quantum Techniques

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This talk provides an overview of computational techniques for studying oxide reliability in nano CMOS transistors. After an introduction to the charge-trapping and detrapping phenomena limiting the MOSFET lifetime, we discuss a hierarchical approach to the simulation of charge transport in the presence of active oxide traps. The computational accuracy and costs of the simulation methods adopted in this hierarchical approach are discussed using novel planar and FinFET transistors as workbench examples (Fig.6). Drift-Diffusion techniques represent the first step of this approach and allow to efficiently studying reliability in the sub-threshold operational regime, where the transistor behavior is mainly electrostatic-dominated (Fig.7a). Monte Carlo techniques represent the second step of our approach, enabling the study of reliability in the ON-state operational regime, where transport effects are fundamental to describe the transistor behavior (Fig.7b). Finally, full-quantum techniques represent the peak of our approach, enabling the study of reliability in presence of quantum confinement (Fig.8).

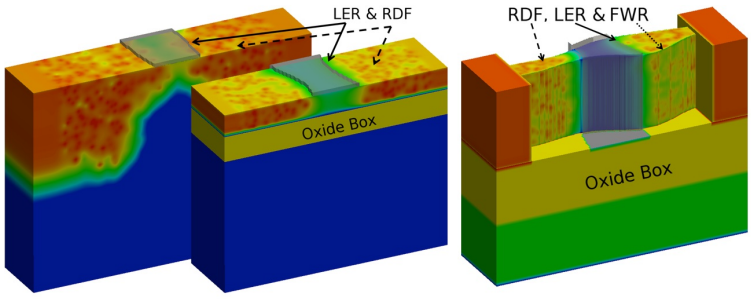

Figure 6: BULK and FDSOI planar transistor (left) and FinFET (right) architectures, showing electron densities at threshold voltage conditions, when affected by statistical variability Random Dopants Fluctuations (RDF), Line Edge Roughness (LER) and Fin Width Roughness (FWR).

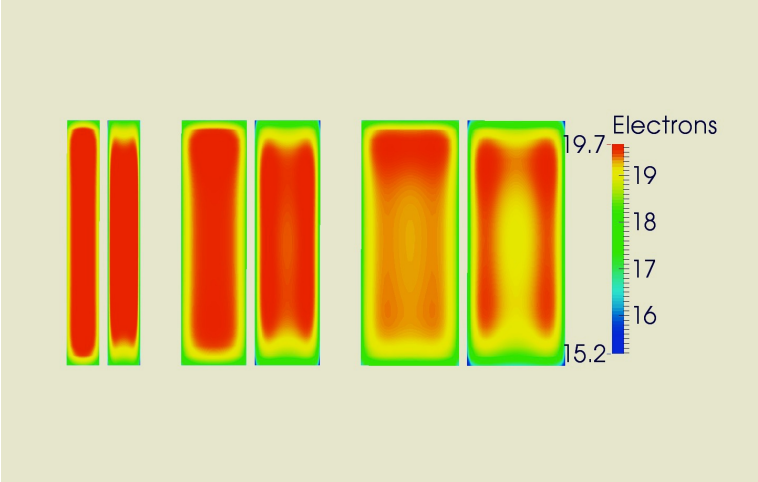

Figure 7: Drift-Diffusion(left) and Schrodinger-Poisson solution of the charge density in a vertical slice at the centre of the channel of a 15nm FinFET transistor. The different charge distributions in the channel will give different reliability performance results.

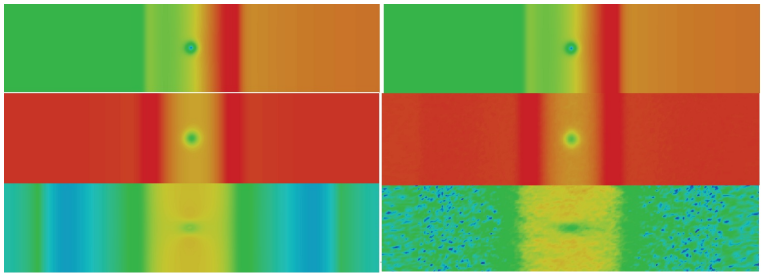

Figure 8: Drift-Diffusion (a. left) and Monte Carlo (b. right) simulation of electrostatic potential (top), electron density (middle) and current density (bottom) showed at 1nm below the channel interface of a planar bulk transistor. A single charge is trapped at the channel/oxide interface in the middle of the channel. The trapped charge in Monte Carlo simulation has an impact not only on the electrostatic but also on the transport (i.e. on charge mobility).

Full-Band Calculations of Thermoelectric Properties of Si Nanowires and Thin Layers

Neophytos Neophytou and Hans Kosina

Author Keywords: thermoelectrics, tight-binding sp3d5s*∗, modified valence-force-field, Boltzmann transport, Seebeck coefficient, silicon ultra-thin layers, silicon nanowires

Abstract

Low-dimensional semiconductors are considered promising candidates for thermoelectric applications with enhanced performance because of a drastic reduction in their thermal conductivity, l, and possibilities of enhanced power factors. This is also the case for traditionally poor thermoelectric materials such as silicon. This work presents atomistic simulations for the electronic, thermal, and thermoelectric properties of Si ultra-thin layers and nanowires of diameters in certain cases up to 20nm. We couple the Linearized Boltzmann theory:

- to the atomistic sp3d5s* tight-binding (TB) model for the electronic properties of the channels, and
- to the modified valence-force-field method (MVFF) for the calculation of their thermal conductivity.

We calculate the room temperature electrical conductivity, Seebeck coefficient, power factor, thermal conductivity, and ZT figure of merit of the ultra-thin Si layers and nanowires. We describe the numerical formulation of coupling TB and MVFF to the Linearized Boltzmann transport formalism, together with all relevant scattering mechanisms. The properties of low-dimensional channels are highly anisotropic, and optimized thermoelectric properties can be achieved by the choice of the appropriate transport and confinement orientations, as well as confinement length scale. We identify bandstructure engineering techniques that lead to thermoelectric power factor improvements. Finally, we show that modulation doping techniques can improve thermoelectric performance significantly.

Electron Momentum and Spin Relaxation in Silicon Films: A Rigorous k p-based Approach

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Growing technological challenges and soaring costs are gradually bringing the MOSFET scaling to an end. This intensifies the search of alternative technologies and computational principles. The electron spin attracts attention as a possible candidate to be used in future electron devices for complimenting or even replacing the charge degree of freedom employed in MOSFETs. The spin state is characterized by the two spin projections on a given axis and it thus has a potential in digital information processing. In addition, only a small amount of energy is needed to flip the spin orientation. Silicon is an ideal material for spintronic applications due to the long spin lifetime in the bulk. The spin lifetime is determined by the spin-flip scattering between the valleys located on different crystallographic axes [1]. This mechanism is suppressed in thin films; however, large spin relaxation in gated silicon structures was observed [2]. Understanding the spin relaxation mechanisms and ways to boost the spin lifetime in confined electron systems is urgently needed.

We investigate the spin relaxation in (001) silicon structures by taking into account surface roughness and electron-phonon scattering. The surface roughness scattering matrix elements are proportional to the product of the corresponding subband wave functions derivatives at each interface

[3]. Electron-phonon scattering is considered in the deformation potential approximation. To find the wave functions and matrix elements we use the effective $\mathbf{k}\cdot\mathbf{p}$ Hamiltonian written at the X-point for the two relevant valleys along the OZ-axis with the spin degree of freedom included [1]. We generalize the deformation potential theory to include the shear strain deformation potential and the deformation potential due to spin-orbit interaction responsible for spin relaxation in confined systems [4].

In the two valleys + two spin projections basis the subband wave functions possess four components. Without spin-orbit interaction included the wave function conserves the spin projection which we assume along OZ-axis for concreteness. The two components corresponding to the up-spin projection are well described by $\psi_{11} = e^{ik_0 z}\sin(\frac{\pi z}{t})$(Fig.9a) and its conjugate corresponding to the usual envelope quantization function located at the valley minima $k_0 = \pm 0.15\frac{2\pi}{a}$. Under shear strain ε_{xy} the degeneracy between the two unprimed subbands is lifted which results in slightly different envelope functions (Fig.9b). The **down-spin** components are proportional to the spin-orbit interaction strength (Fig.10a). Under shear strain ε_{xy} these components are greatly suppressed (Fig.10b). As a confirmation of the Elliot-Yafet spin relaxation mechanism, the spin lifetime is proportional to the momentum relaxation time (Fig.11a). Under shear strain ε_{xy} the spin lifetime is enhanced much stronger than the mobility (Fig.11b) due to the **down-spin** components suppression (Fig.10b). In conclusion, shear strain boosts both electron mobility and the spin lifetime in silicon films.

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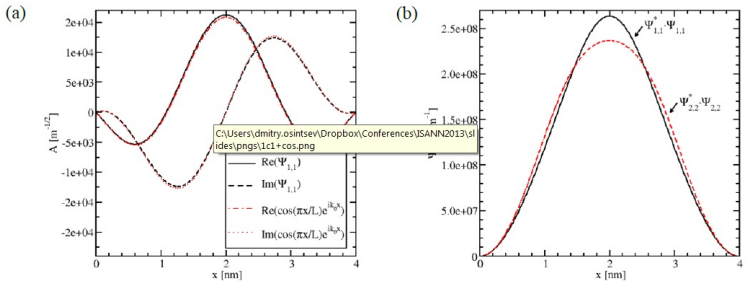

Figure 9: (a): The up-spin component of the wave function of the lowest unprimed subband in unstrained film located in the valley centered at k_0 (b): The up-spin components of the two unprimed subbands with ε_{xy}0.05%

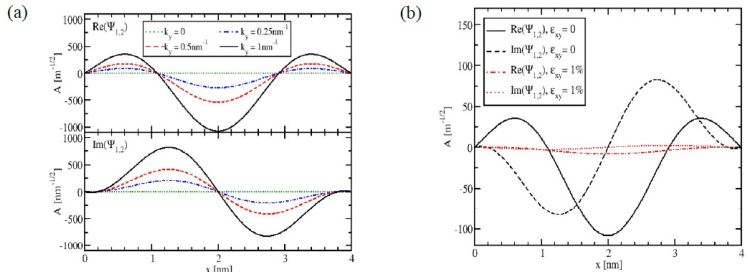

Figure 10: (a): The down-spin components are proportional to the strength of the spin-orbit interaction (b): The down-spin components are considerably suppressed by tensile shear strain

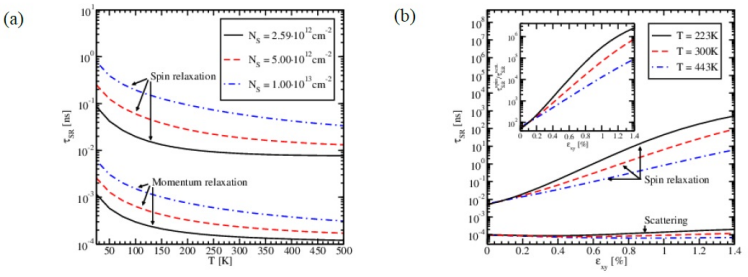

Figure 11: (a): The spin lifetime is proportional to the momentum relaxation time as function of temperature. This is an indication of the Elliot-Yafet spin relaxation mechanism [1] (b): Spin lifetime and momentum relaxation time enhancement with tensile shear strain. Inset: ratio of the spin to the momentum relaxation time

Drift-Diffusion Models for Organic Photovoltaics: Deriving a Unipolar Model

Daniel Brinkman, Klemens Fellner and Peter Markowich

Author keywords: Drift Diffusion Modeling, Organic Photovoltaics, Asymptotic Analysis

Abstract

Drift-Diffusion equations have long been used with great success for semiconductor devices. With the advances in new organic materials, it becomes crucial to extend our inorganic semiconductor modeling to organic devices. The main challenge is the inclusion of two distinct materials: an electron-donor and an electron-acceptor. Due to the different Fermi levels in the device, it is sensible to consider the limit where the electron-donor contains only holes and the electron-acceptor contains only electrons. Further assuming a donor-acceptor interface of width zero allows for explicit solutions in 1D (up to suitable boundary conditions at the donor-acceptor interface).

For most organic devices, current generation only occurs at the interface between the two materials (as the single-particle band-gap for the materials is large). As such, it becomes incredibly important to model the interface of the device. The boundary conditions can be artificially constructed to retain important physical quantities, but we then run the risk of losing information about the dynamics of the interface. Thus our goal is to obtain the unipolar model through a consistent limit of the finite interface model with two charge carriers. However, we will show that simple methods for

taking this limit generally either violate conservation of current or admit an open-circuit state for which the hole and electron currents are both nonzero.

Neumann Series Analysis of the Wigner Equation Solution

Ivan Dimov, Mihail Nedjalkov, Jean Michel Sellier and Siegfried Selberherr

Author keywords: Quantum transport, Wigner function, Integral equation, Neumann series.

Abstract

The existence and uniqueness of the electron transport Wigner equation solution, determined by boundary conditions is analyzed in terms of the Neumann expansion of the integral form of the equation, obtained with the help of Newton's trajectories. For understanding of the peculiarities of Wigner-quantum electron transport in semiconductor structures such mathematical issues can not be separated from the physical attributes of the solution. In the presented analysis these two sides of the problem mutually interplay. The problem is first formulated from a physical point of view, where the stationary solution is considered as the long time limit of the general evolution problem posed by both initial and boundary conditions.The proof of the convergence relyes on the assumption for reasonable local conditions which may be specified for the kernel and on the fact that the Neumann expansion corresponds to an integral equation of Volterra type with respect to the time variable.

Strategies to improve the control of current in graphene transistors

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As a high mobility material, graphene is well suited for high frequency electronics [1]. However, the absence of bandgap restricts the switching-off capability of graphene transistors, which even for microwave applications is a problematic limitation. Actually, in conventional pristine graphene transistors, the switching-off of current at low gate voltage (npn configuration) is prohibited by the onset of (chiral) Klein tunnelling [2] which makes it possible for particles on electron states in the source to propagate through the hole states of the gated portion of the channel with a high transmission coefficient. It also degrades the saturation of the drain current, leading to a huge output conductance that impairs the maximum oscillation frequency f_{max}. Different strategies may be envisioned to overcome this issue. We will review and discuss three of them, essentially by means of simulation results obtained from tight-binding/Green's function approach of transport.

The first idea may be to suppress the Klein tunnelling by generating a bandgap in graphene to restore conventional properties of field-effect transistors. It has been suggested for instance to cut a graphene sheet into nanoribbons [3], to apply an electric field perpendicular to a bilayer graphene sheet [4], to use nitrogen-doped graphene [5] or to exploit the Bernal stacking of graphene on hexagonal boron nitride substrate [6]. We will focus on the possibility to open up a band gap in a large sheet of graphene by punching

a high-density array of periodic nanoholes to form a graphene nanomesh [7]. It allows improving strongly the device characteristics though the carrier mobility and the on-state current are reduced. We will also discuss the possibility of tuning the bandgap of graphene/BN ribbons using a transverse electric field.

The second idea is based on the strain engineering of graphene sheets [8]. Though a small strain does not open any bandgap in the electronic structure, we will show how an appropriate strained/unstrained graphene junction leads to a large conductance gap thanks to the shift of Dirac points between strained and unstrained portions of graphene. It may lead to the strong suppression of Klein tunnelling and to improved device performance.

Finally, we will discuss the opportunity offered by the Klein tunnelling effect of ballistic Dirac fermions (DFs) in graphene. In this transport regime, DFs manifest optics-like properties at interfaces determined by Fresnel-like relations. We show that in a pnp transistor that exploits the internal reflection in a Klein tunnelling prism made of an n-doped triangular area controlled by a triangular gate, the transmission is suppressed when increasing the gate doping deep in the metallic regime, in strong contrast with conventional semiconducting transistors [9]. It allows suppressing the current much below the current at the Dirac point, without making use of any bandgap, while the on-current remains high.

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Simulation, Model Order Reduction and Robust Optimization for Industrial E-Mobility Applications

HJB-POD feedback control for Navier-Stokes equations

Alessandro Alla and Michael Hinze

Author keywords: Optimal Control, Proper Orthogonal Decomposition, Hamilton-Jacobi equations, Navier-Stokes equations

Abstract

We consider the approximation of an infinite horizon optimal control problem for an evolutive partial differential equation. The method is based on a model reduction technique, using a POD approximation, coupled with a Hamilton-Jacobi equation which characterizes the value function of the corresponding control problem for the reduced system. Although the approximation schemes available for the HJB are shown to be convergent for any dimension, in practice we need to restrict the dimension to rather low number (typically 4) and this limitation affects the accuracy of the POD approximation. We will present numerical tests for the control of the time-dependent Navier-Stokes system with two-dimensional spatial domains to illustrate our approach and to show the effectiveness of the method.

Uncertainty Quantification of geometric and material properties of permanent magnetic synchronous machines

Zeger Bontinck, Herbert De Gersem and Sebastian Schoeps

Author Keywords: Uncertainty Quantification, PMSM, Eccentricity

The behaviour of electrical machines is accurately predicted by finite element simulations. During the design phase, parameter studies and optimization steps are carried out but rarely sensitivities are analysed. However, manufacturing imperfections and uncertain operating conditions are unavoidable. The quantification of their impact on the machine parameters and operation performance can help to increase the robustness of the machine. Accordingly, methods for sensitivity analysis are getting more and more attention.

In this research a 6-pole permanent magnetic synchronous machine is studied by using uncertainty quantification. The uncertain parameters taken into account are related to the geometric properties of the machine (e.g. eccentric rotor positions) or to the material properties (e.g. anisotropic magnets). In order to determine the most sensitive parameters, the influence is studied on the higher harmonic air-gap field components of the machine by using a Monte-Carlo approach. The geometric variations are modelled without remeshing the finite element triangulation in order to avoid numerical noise caused by meshing in the stochastic outputs.

It is found that eccentricity increases the total harmonic distortion. If

the rotor's centre is described by polar coordinates with respect to the stator's centre, the radial component has more influence on the total harmonic distortion than the angular component.

Analysis of the Contraction-Condition in the Co-Simulation of a Specific Electric Circuit

Kai Gausling and Andreas Bartel [109]

Abstract

Co-simulation is an important method for coupled systems in time domain. In particular, if the monolithic description of a dynamic system is not feasible and/or dedicated simulation tools for the subsystems are available, then it is relevant option. Using the co-simulation methodology, one has a tool at hand, which is capable of multirate, multimethod, multiorder (and so on).

However, convergence can only be achieved by solving multiple times the subsystems. To enhance convergence, the whole simulation time is split into time windows. In fact, co-simulation applied to coupled ordinary differential equations always convergences. But the situation is different for coupled differential algebraic equations. In the latter case convergence can only be guranteed if certain contraction properties are given, see e.g. [1], [2]. It can be shown that the convergence and stability of cosimulation is directly influenced by the coupling interface, see e.g. [3]. Usually the contraction condition itself is obtained by some estimations. This paper takes a closer look at the coupling structure of a simple electric circuit. Using standard

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theory for the example, no contraction would be inferred. However, co-simulation converges. By a detailed analysis, we can prove convergence in this case.

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Parameter identification for nonlinear elliptic-parabolic systems with application in lithium-ion battery modeling

Oliver Lass

Author Keywords: Nonlinear elliptic-parabolic systems, Optimization with PDE constraints, Parameter estimation, Model order reduction, Proper orthogonal decomposition.

Abstract

Recently the modeling and simulation of lithium-ion batteries has gained a lot of interest in many scientific and industrial fields. In this talk generalized mathematical systems arising from the modeling of lithium-ion batteries are considered. The investigated model is expressed in terms of two elliptic and one parabolic partial differential equations (PDEs) that are highly nonlinear and coupled. These equations describe the concentration of lithium ions and the potential in the solid and liquid phases. There are several parameters in the PDE system which are not known a-priori or which cannot be determined experimentally. To calibrate the model, efficient numerical algorithms to estimate unknown parameters are needed. For this purpose the parameter identification problem is formulated as a nonlinear least-squares problem. To investigate the parameter depending behavior of the nonlinear system output a sensitivity analysis is carried out. By utilizing a subset selection method the relevant parameters for the optimization process are determined. To speed up the optimization algorithms a model reduction approach based

on proper orthogonal decomposition (POD) is applied. Numerical examples will be presented to illustrate the efficiency of the proposed methods.

Structured Numerical Linear Algebra in Imaging and Monument conservation

Multigrid Regularization Method for image deblurring with arbitrary boundary conditions

Alessandro Buccini and Marco Donatelli

Author keywords: Image deblurring, Multigrid, Inverse problem.

Abstract

In many applications, such as astronomy and medicine, arises the problem of deblurring images, this inverse problem is ill-conditioned and the inevitable presence of noise make a very dicult task obtain- ing a good reconstruction of the true image. Recent results have shown that iterative methods of multigrid type are very precise and ecient for regularizing purposes. We want to combine this multigrid methods with framelet denoise; the multigrid will regularize and solve the prob- lem and the denoise will be used for keeping under control the eect of noise going on with the iterations. For pre-smoothing we will use conjugate gradients for normal equations and preconditioned iterative methods for ill-posed problems. The resulting regularization multigrid method shows a fast and stable convergence.

A crucial issue with the deblur problem is the treatment of bound- ary artefacts (ringing eects), we will consider dierent types of bound- ary conditions and we will use a particular technique that let us avoid them at all. Finally we will compare the results with the dierent approaches.

This is a joint work with Marco Donatelli from Universita degli Studi dell'Insubria.

Data based regularization methods

Thomas Huckle

Author keywords: Inverse ill-posed problems, Regularization, Seminorm, Preconditioning

Abstract

We focus on the solution of discrete deconvolution problems to recover the original information from blurred signals in the presence of Gaussian white noise more accurately. For a certain class of blur operators and signals we develop a diagonal preconditioner/seminorm to improve the reconstruction quality, both for direct and iterative regularization methods. In this respect, we incorporate the variation of the signal data during the construction of the preconditioner. Embedding this method in an outer iteration may yield further improvement of the solution. To estimate the optimal number of iterations in connection with (P)CGLS, we provide a comparison between different L-curve approaches, especially based on B-splines, and the Discrepancy Principle. Furthermore, we introduce operator dependent seminorms for Tikhonov-Phillips regularization. Reconstructions of numerous discrete ill-posed model problems, arising both from realistic applications and examples generated on our own, demonstrate the effect of the presented approach.

Multigrid preconditioning for nonlinear (degenerate) parabolic equations with application to monument degradation

Marco Donatelli[110], Matteo Semplice[111] and Stefano Serra-Capizzano[112]

Abstract

We consider linear systems of large dimensions, (locally) structured, resulting from the linearization of systems of nonlinear equations obtained by discretizing nonlinear parabolic equations (possibly degenerate) by means of finite differences in space and implicit schemes in time. In the first part, we consider a uniform discretization in space. Using the theory of sequences of (locally) Toeplitz matrices for studying the spectrum of the Jacobian matrix of Newtons method, we prove the convergence and we derive optimal preconditioners based on multigrid techniques. The numerical tests are conducted on the equation of porous media and on a particular nonlinear

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parabolic equation that models the sulfation of marble by polluting agents [1, 3]. Subsequently, driven by the presence of a boundary layer in the model of sulfation, we extend the previous results to the case of not uniform grids in space, using preconditioners based on algebraic multigrid [2].

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A free-boundary model of corrosion

F. Clarelli, B. De Filippo and R. Natalini[113]

Abstract

Deterioration of copper and bronze artifacts is one of the main concerns for people working in cultural heritage. In particular a significant effort has been devoted to study the corrosion due to environmental conditions, such as temperature, moisture and the concentration of pollutants. We introduce a mathematical model able to describe the corrosion effects on a copper layer, which is subject to deposition of SO_2. The present model is based on a partial differential equation system with a double free boundary for monitoring and detecting copper corrosion products (mainly brochantite and cuprite).We assume to have a copper sample on which is formed a non protective oxide layer (Cu_2O), and, over this layer, a corrosion product (brochantite) grows. We aim to create a new approach to forecasting corrosion behavior without the necessity of an extensive use of laboratory testing using chemical-physical technologies, while taking into account the main chemical reactions. Although the model was kept simple, just describing the main reaction and transport processes involved, the mathematical

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simulations and the related model calibration are in agreement with the laboratory experiments.

Keywords: Free boundary model, parabolic problems, finite difference methods, corrosion, copper, brochantite, cultural heritage

MSC 76V05, 35R35, 65M06

Numerical methods for nonlinear PDEs modeling monument preservation

Armando Coco, Marco Donatelli and Matteo Semplice

Author Keywords: nonlinear PDEs, marble sulfation, level set, ghost points methods, finite differences.

Abstract

Marble monument sulfation consists in the formation of gypsum crusts by the degradation of the outer layer of stone, due to the aggression of sulfates in humid environments. [1] describes a mathematical model for this phenomenon and validated it with experiments of accelerated degradation in the lab. Numerical predictions can be achieved, in simple geometries with finite difference methods [2,3], but for more realistic situations it is a challenging task. Aftre a brief survey, in this talk I will concentrate on numerical discretizations that can deal with the complex geometries that characterize real monuments. In particular, I will consider an approach where the computational domain is described by a level-set function defined on a (uniform) cartesian grid. The nonlinear parabolic PDEs of the model are discretized by finite differences and boundary conditions are applied with a ghost-point strategy that was succesfuly employed in elliptic PDEs [4].

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Mathematical Problems from Semiconductor Industry

Fast Fault Simulation to identify subcircuits involving faulty components

B. Tasić, J.J. Dohmen, E.J.W. ter Maten, T.G.J. Beelen, W.H.A. Schilders
[114]

Abstract

Imperfactions in manufacturing processes may cause unwanted connections (faults) that are added to the nominal, *golden*, design of an electronic circuit. By fault simulation we simulate all situations: new connections and each with different values for the newly added element. During the transient simulation the solution of a faulty circuit is compared to the golden solution of the fault-free circuit. A strategy is developed to efficiently simulate the faulty solutions until their moment of detection. We fully exploit the hierarchical structure of the circuit in the simulation process to bypass parts of the circuit that appear to be unaffected by the fault. Accurate prediction and efficient solution procedures lead to fast fault simulation in which the golden solution and all faulty solutions are calculated over a same time step. Finally, we store a database with detectable deviations for each fault. If such

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a detectable output *matches* a measurement result of a product that has been returned because of malfunctioning it helps to identify the subcircuit that may contain the real fault [1].

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Charge transport in OLETs: mathematical model and numerical simulations

Paolo G. Ferrandi, Stefano Micheletti and Paolo Simioni

Author Keywords: Organic semiconductors, Drift-Diffusion equations, BOX discretization method.

Nanotechnology has increasingly affected our daily life. Generally, the scale ranges from 1 to 100 nanometres. The applications of nanotechnology can cover many areas in our lives, and one of the applications is light emitting devices. For instance, inorganic semiconducting crystalline nanowires made from III-V materials have been investigated to fabricate nanowire field-effect transistors , multicolor light sources, lasers, photo detectors and solar cells based on their well-defined properties.

Recently high performance electric and optoelectronic devices based on organic semiconductors have also been demonstrated, such as organic light emitting diodes (OLED), field-effect transistors (FETs), and solar cells. These organic devices show promise for low-cost, large-area and flexible devices. In particular, display panels using OLED are expected for mobile electronic devices and excellent stability and high efficiency OLED have been reported.

On the other hand, rapid progress of organic light-emitting field-effect transistors (OLEFETs) has been made in recent years. An organic light-emitting transistor (OLET) is a form of transistor that emits light. These transistors have been claimed to have potential for digital displays and on-chip optical interconnects. OLET is a new light-emission concept, providing planar light sources that can be easily integrated in substrates like silicon, glass, paper using standard microelectronic techniques.

In this communication, we present the mathematical model that we have devised for describing charge transport in OLETs for industrial applications. This model is based on the standard Drift-Diffusion equations, plus singlet and triplet exciton formation. Discretization is based on a BOX method suitably devised for regular tetrahedra. Fully 3D numerical simulations assess the performance of the overall method.

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Index-aware Model Order Reduction methods for electrical networks

Giuseppe Ali, Banagaaya Nicodemus and Schilders W.H.A.

Author Keywords: differential algebraic equations, tractability index, model order reduction, modified decomposition of DAEs.

We present a class of model order reduction (MOR) methods for differential-algebraic equations, which are based on the intrinsic differential equation contained in the starting system and on the remaining algebraic constraints. The decoupling procedure in differential and algebraic part is based on the projector and matrix chain which leads to the definition of tractability index. The differential part can be reduced by using any MOR method, in particular we use Krylov-based projection methods to illustrate our approach. The reduction on the differential part induces a reduction on the algebraic part. In this talk, we present the method for arbitrary index differential-algebraic equations. We also present an implicit version of the same MOR procedure. We implement numerically these procedures and show numerical evidence of their validity.

Multirate GARK schemes for coupled problems

Michael Günther, Christof Hachtel and Adrian Sandu.

Author Keywords:Coupled problems, Runge-Kutta schemes, Multirate GARK schemes.

Abstract

Multirate GARK schemes define a multirate extension of GARK schemes, generalized additive Runge-Kutta schemes. These allow for exploiting multirate behaviour in both the right-hand sides and in the components in a rather general setting, and are thus especially useful for coupled problems.

In this talk, we will derive Multirate GARK schemes and discuss their main properties: convergence and order conditions, as well as linear and nonlinear stability properties. Numerical results for coupled test problems will be discussed.

Numerical Methods in Volcano Geophysics

Fictitious domain methods for fracture models in elasticity

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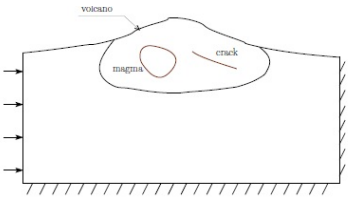
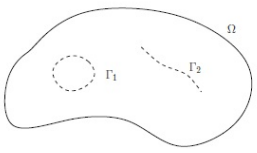
The aim of this work is to carry out a generic method for imposing jump conditions across interfaces (cracks for instance) whose the geometry would likely evolve through the time or more generally during iterations. The robustness with respect to this geometry is an important criterion, since the underlying purpose lies in solving inverse problems for which the geometry and the position of the crack is the unknown. That is why we consider a *fictitious domain* method, with which the mesh of the computational domain is independent of the crack.

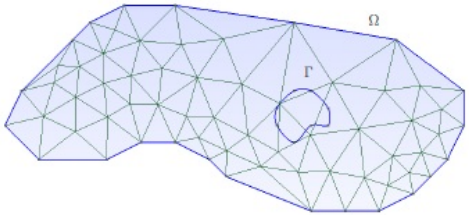
In order to illustrate this approach, we consider a linearized elasticity problem governing the displacement inside a volcano submitted to internal cracks. The presence of these cracks induces jump conditions that we have to taken into account.





Denoting by $\mathbf{u}$ the displacement inside the computational domain, and by $\sigma_L(u) = \mu_L(\nabla\mathbf{u} + \nabla\mathbf{u}^T) + \lambda_L(\div\mathbf{u})\mathbf{I}_{\mathbb{R}^d}$ the Lamé stress tensor (with $d = 2$ or 3), the linear elasticity problem we consider is the following

$$\begin{cases} -\text{div } \sigma_L(\mathbf{u}) = f & \text{in } \Omega, \\ \mathbf{u}_{|\partial\Omega} = g & \text{on } \partial\Omega, \\ [\mathbf{u}] = D & \text{on } \Gamma, \\ [\sigma_L(\mathbf{u})n] = 0 & \text{on } \Gamma. \end{cases}$$



The quantities f, g, D are given data, and $[\cdot]$ denotes the jump of a vector field across the crack Γ. Of course, mixed boundary conditions can be imposed on $\partial\Omega$ instead of the Dirichlet condition we consider here. Several strategies will be presented, underlined by convergence curves and consideration of different types of geometries. They are based on non-conforming meshes, that is to say meshes which do not match to the geometry of the crack.

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Multi-Objective Optimization, Sensitivity and Robustness Analyses for the inverse modeling of Ground Deformation and Gravity Changes of the 1981 Etna Eruption

Giuseppe Nicosia, Piero Conca, Jole Costanza, Giovanni Carapezza, Gilda Currenti and Ciro Del Negro

Author Keywords: Computational Geophysics, Geodesy and Gravity: Gravity anomalies and Earth structure, Geodesy and Gravity: Transient deformation, Volcanology: Eruption mechanisms and flow emplacement, Volcanology: Volcano monitoring, Multi-Objective Optimization, Sensitivity Analysis, Robustness Analysis, ground deformation, gravity changes.

In recent years the inverse modeling of geophysical observations have improved our understanding of volcanic processes. Mt Etna is one of the most monitored volcanoes worldwide and represents a natural laboratory, which provides a multi-parametric array of geophysical datasets to be exploited for the advancement and validation of new modeling inversion algorithms and analysis. This paper analyses a model described in [1], which interpret the data collected during the 1981 eruption of Mt Etna using multi-objective and single-objective optimization for the inverse modeling. The model results

indicates that the 1981 eruption was generated by a magmatic intrusion, which opens up new fractures and fills preexisting micro-cracks. Single-objective optimization and multi-objective optimization are here applied to that model in order to find additional and potentially better solutions. The used techniques are the genetic algorithm NSGA2 and the differential evolution (DE). The solutions provide a better fitting of the model to the geophysical observations with respect to the previous results. In particular, NSGA2 shows lower fitting error in EDM, levelling and micro-gravity measurements; while the DE algorithm provides lower errors for the first two measures with respect to NSGA2. The sensitivity of the models to variations of their parameters are investigated by means of the Morris method with the aim of identifying the parameters that have higher impact on the model. In particular, these model parameters control the position of the sources, their dip and the porosity of the infiltration zones. In addition, being the robustness a good indicator of the quality of a solution [2], a subset of configurations with good characteristics is selected and their robustnesses is evaluated in order to identify a suitable model.

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Geophysical changes in hydrothermal-volcanic areas: A Second Order Finite-Difference Ghost-Cell Method to solve thermo-poro-elastic equations

Armando Coco, Gilda Currenti, Ciro Del Negro, Joachim Gottsmann and Giovanni Russo.

Author Keywords: Hydro-thermal volcanic processes, geophysical modeling, thermo-poroelastic equations.

The increasing combined use of long-term InSAR time-series and ground-based geophysical observations in volcanic areas has dramatically enhanced our ability to detect and track complex and multifaceted volcanic processes that are often difficult to reconcile using models of elastic mechanical behaviour of Earth's upper crust. Usually, magma accumulation and intrusion are modelled as volume and pressure changes induced by magma migration. However, the interaction between magma and host rocks such as the heating and expansion of hydrothermal fluids also induces measurable changes in geophysical signals. Although hydrothermal processes have been discussed as possible causes of volcano monitoring signals, few studies have addressed the quantification of the expected changes associated with thermal expan-

sion and pore pressure changes. A thermo-poro-elastic numerical model is proposed to jointly evaluate ground deformation, magnetic and gravity changes caused by hydrothermal pressurization in complex media with surface topography and mechanical heterogeneities. The aim is to provide a numerical framework for a more realistic assessment of stress and strain partitioning associated with sub-volcanic processes.

New progress on numerical modeling of Geophysical flows for environment, natural hazards, and risk evaluation

Well-Balanced Schemes for the Shallow Water Equations with Coriolis Force

Alina Chertock, Michael Dudzinski, Alexander Kurganov and Maria Lukacova-Medvidova

Author Keywords: shallow water equations Coriolis force second order reconstruction well-balanced methods hyperbolic balance laws central upwind schemes finite volume evolution Galerkin schemes jets in the rotational frame

Abstract

In this talk, we will discuss shallow water equations with the bottom topography and Coriolis force. The later yield nonlocal potential operators that need to be taken into account in order to derive a well-balanced numerical scheme. In the presence of the Coriolis force, the structure of the steady-state solutions becomes very complex as the governing system of equations admits not only the *lake at rest* steady states, but also geostrophic equilibria, near which the circulations are observed.

A crucial step in the construction of high-order approximations for the underlying systmes is a well-balanced reconstruction which has to be combined with the well-balanced update in time. We introduce a quite general reconstruction procedure that can be used in conjunction with a variety of numerical schemes. Theoretical proofs and numerical experiments clearly demonstrate that the resulting numerical methods are well-balanced.

Simulations of 3d Navier-Stokes equations with free surface for hydrodynamics-biology coupling and marine energies

Marie-Odile Bristeau, Raouf Hamouda and Jacques Sainte-Marie

Author Keywords: Free surface flows, Navier-Stokes equations, Geophysical flows, Hydrodynamics-biology coupling, Renewable energies

Abstract

Gravity driven geophysical flows are usually represented by the incompressible Navier-Stokes or Euler equations with free surface.
Because of the scales in space and time of the considered problems, simpler models like shallow water type models (Saint-Venant system) are often used to model phenomena such as rivers, coastal domains, oceans or even run-off or avalanches when being modified with adapted source terms.

However, the scientific challenges, the breakthroughs and the real-life applications concern complex phenomena and flows for which more accurate models than the Saint-Venant system are required. In this presentation, we present a robust and efficient technique for the numerical simulation of the incompressible 3d hydrostatic Navier-Stokes equations with free surface.

To illustrate the abilities of the numerical technique and code, we present several application examples concerning hydrodynamics-biology coupling for algae culture and biofuel production and also water depollution.

A multilayer approach for the simulation of suspended sediment transport

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Keywords: multilayer shallow water, turbidity currents, finite volume schemes.

Abstract

Sediment can be transported in several ways by the action of a river. During low transport stages, particles move by sliding and rolling over the surface of the bed. With the increase of the velocity, the sediment is entrained into suspension and travels significant distances before being deposed again. One can observe a continuous exchange between sediment at the river bed and sediment in suspension. Moreover, when the concentration of suspended sediment is elevated, the river can plunge into the ocean creating a hyperpycnal plume.

One possible approach to model these phenomena is to use a shallow water model coupled with transport equations for sediment in suspension and a morphodynamical component for the bedload transport, which depends on an empirical flux. This was in fact the approach used in [3].

One can prove that this system is hyperbolic at least for most physical situations. The model can be also completed in order to take into account gravity effects as it was done in [2].

The drawback of this model is that it only takes into account the mean depth-average concentration of each sediment specie in suspension and as a consequence we lose the vertical distribution of sediment within the fluid. The characteristic behavior of a mixture of fluid and suspended small particles, which belong to a finite number of species differing in size or density, leads to areas of different composition and this information could be relevant in practical applications.

Following the ideas presented in [1], we propose here to derive a model that extends the model presented in [3] and includes information on the vertical distribution of particles. To do so, we divide the hyperpycnal plume in M layers with thickness h_α and horizontal velocity $u_\alpha, \alpha = 1, \ldots, M$ (see Figure). Within each layer α, we shall consider N different sediment species and denote $\phi_\alpha, i = 1, \ldots, N$ the mean average of its volumetric concentration in this layer. This will give us a vertical distribution of the particles provided that the number of layers M is large enough. In order to solve numerically the problem, a two-step algorithm is proposed. First, horizontal motion of the fluid is carried out. Then, a numerical scheme adapted for the sedimentation of particles is applied in the vertical direction. This vertical motion of particles can be generalized by using polydisperse sedimentation models as it is described in [4]. Numerical simulations with this new model show interesting profiles of suspended sediments that will not be observed otherwise and are expected to be in better agreement with practical applications.

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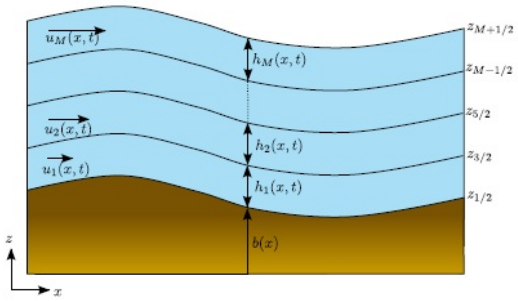

Figure 12: Sketch of a multilayer fluid

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Modelling and numerical approach of viscoplastic avalanches

Enrique Fernandez-Nieto, José María Gallardo Molina and Paul Vigneaux

Author keywords: Avalanches, Viscoplastic, Duality methods, Well-balanced.

Abstract

In this work we study the numerical approach of several types of shallow viscoplatic models with application in risk evaluation of avalanches. Several types of models will be considered. First, we see that they can be written under a common structure, in form of variational inequality. To discretize these type of models we consider two types of duality methods - Augmented Lagrangian and Bermdez Moreno- combined with finite volume methods. A special treatment of the multiplier must be taken into account in order to obtain well-balanced finite volume solvers. Moreover, we present a generalization of the wet/dry numerical treatment that was first introduced for the case of Shallow Water equations. Finally, some numerical tests will be presented.

Well-balanced schemes for Shallow-Water models with strongly non-linear source terms

Christophe Berthon

The present work is devoted to the derivation of accurate finite volume schemes to capture sophisticated steady states issuing from shallow-water models supplemented by strongly non-linear source terms. Two distinct models are here considered. The first one is the Ripa model [1,5] to take into acount the temperature potential within the flow. The second model under consideration is the shallow-water model with Manning friction. Both models involve very sophisticated steady states which are of prime importance for simulations. When compared to the well-known shallow-water model, the here considered steady states are not explicitly given. For instance, the steady states associated to the shallow-water model with Manning friction are solution of a strongly non-linear algebraic relation. In the case of the Ripa model, the steady states are solutions of a non-solvable partial differential equation.

To approximate the solutions of these systems, we adopt finite volume methods deriving from Godunov-type schemes [3]. Because of the source terms, the celebrate Harten, Lax and van Leer result [3], cannot be directly applied. However, after [2], the source term average can be easily introduced within an approximate Riemann solver to get consistent schemes. Next, the main idea consists in electing a suitable source term average in order to recover the required well-balanced property [6]; namely to exactly capture the steady states of interest. Considering the shallow-water model with

Manning friction, we obtain an approximate Riemann solver which exactly capture the solution of the non-linear equation governing the steady states. Let us underline that we get a well-balanced scheme witout solving the steady states.

Concerning the Ripa model, the situation turns out to be distinct since the steady states of interest are governed by a partial differential equation. Here, we exhibit three classes of solutions to be exactly captured by the scheme (in [1] just two classes are considered). The required well-balance property is, once again, obtained by adopting a relevant source term average within the derived approximate Riemann solver. The resulting scheme is thus proved to exactly capture the exhibited classes of steady states. Moreover, the scheme approximate, in a sense to be specified, partial differential equation governing the steady states. It is worth noticing that the derived approximate solvers preserves additional crucial properties (robustness and stability).

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Path-Conservative Central-Upwind Schemes for Nonconservative Hyperbolic Systems

Manuel Jesus Castro Diaz, Yuanzhen Cheng, Alina Chertock, Alexander Kurganov and Tomas Morales de Luna

Author Keywords: Nonlinear hyperbolic systems, nonconservative products, central-upwind schemes, path-conservative schemes, Saint-Venant system of shallow water equations, two-layer shallow water equations, two-mode shallow water equations.

I will present a new path-conservative central-upwind scheme for nonconservative hyperbolic systems of PDEs. Such systems arise in a variety of applications and the most challenging part of their numerical discretization is a robust treatment of nonconservative product terms.

Godunov-type central-upwind schemes were developed as an efficient, highly accurate and robust "black-box" solver for hyperbolic systems of conservation laws. They were successfully applied to a large number of hyperbolic systems including such nonconservative systems as two-layer shallow water equations, compressible two-phase flow models, Savage-Hutter type system modelling submarine underwater slides. To overcome the difficulties related to the presence of nonconservative product terms, several special techniques were proposed. However, none of these techniques was sufficiently robust and thus the applicability of the original central-upwind scheme was quite limited.

We have recently realized that the main drawback of the original approach was the fact that the jump of the nonconservative product terms

across cell interfaces has never been taken into account. Rewriting central-upwind schemes in the form of path-conservative schemes has helped to understand how the nonconservative products should be discretized so that their influence on the numerical solution is accurately taken into account. The resulting path-conservative central-upwind scheme is a new robust tool for both conservative and nonconservative hyperbolic systems. The new scheme has been applied to the Saint-Venant system with discontinuous bottom topography, two-layer shallow water system, and the two-mode shallow water equations which was recently derived as a simplified model tat describes nonlinear dynamics of waves with different vertical profiles. Our numerical results illustrate a superb performance of the new path-conservative central-upwind scheme, its robustness and ability to achieve very high resolution.

Some results on the numerical treatment of Movable Bed Shallow Water Equations

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*Keywords:*Shallow Water Equations, Sediment Transport, Movable Bed, Non-conservative Hyperbolic Systems.

Abstract

In this work a preliminary analysis is carried out, concerning the numerical integration of shallow water equations on movable bed. The fundamental aim is to understand if it is possible to capture the main features of some typical meso-scale bedforms, namely river dunes and/or antidunes, through a depth averaged approach, avoiding the numerical integration of full Navier-Stokes Equations by means of RANS or LES approach.

The analysis regards the typical range of fluvial hydraulics, that is low sediment transport rate and negligible collisional effects between solid grains. The governing eqautions are the mass and momentum balance in the shallow water frame and the Exner equation for the bed elevation. Some classical results, considered as stated by the literature on this topic, are taken into account, namely the effects of the skin fiction and of the local bottom slope on the sediment mobility, the key parameter to evaluate the bed load transport.

A source of uncertainties is the separation between the form drag effect and the skin friction effect in evaluating the total friction in a bedform-covered alluvial bottom. In order to separate such effects, we remove the average longitudinal bed slope from the momentum equation, and it is idealized as the external forcing which establishes the average mean flow in the considered domain.

Firstly, a quasi-analytical approach is adopted, considering as small the sediment discharge with respect to the liquid discharge. The flux matrix eigenvalues and eigenvectors are found, and it is shown how sediment transport affects bedforms celerity and Riemann invariants.

Secondly, a relaxation approach is proposed, to take properly into account the bedload time-adaptation to the local hydrodynamic conditions.

In both cases, numerical computations are carried out using the Dumbser-Toro extension of the Osher Riemann Solver to non-conservative hyperbolic systems, in order to properly take into account the role of the bottom elevation as time-space variable. Some examples are shown, in typical range of existence of real river bedforms.

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The randomized level set method and an associated reaction-diffusion equation to model wildland fire propagation

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Abstract

Front propagation is studied in literature by two alternative approaches, namely the reaction-diffusion equation [4] and the level set method [3]. These two approaches are considered alternative each other because the solution of the reaction-diffusion equation is generally a continuous smooth function that has an exponential decay and an infinite support, while the level set method, which is a front tracking technique, generates a sharp function with a finite support. However, these two approaches can indeed be considered complementary and reconciled. When front propagation occurs in a random

environment the front gets a random character, too. Hence the level set contour is here randomized accordingly to the probability density function of the interface particle displacement. The resulting averaged process emerges to be governed by an evolution equation of the reaction-diffusion type [1]. The application of this method to wildland fire propagation is shown [2]. This approach turns out to be useful to simulate effects due to turbulent convection and fire spotting. In particular, the resulting model emerges to be suitable to simulate fire flank and backing fire, the enhancement of fire spread because of the actions by hot air pre-heating and by ember landing, and also the fire overcoming a fire-break zone that is a case not resolved by models based on the level set method.

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2D GPU-based HySEA model for tsunami simulation. Some practical examples

José M. González Vida, Manuel J. Castro, Jorge Macías, Marc de La Asunción, Sergio Ortega and Carlos Sánchez-Linares

Author Keywords: Finite Volume Schemes, Shallow-Water equations, WAF type numerical schemes, GPU based models, Geophysical flows simulation, Tsunami simulation.

A two-waves TVD-WAF type scheme for solving 2D shallow-water equation is considered together with a first and second order HLL scheme. Comparison among the different schemes will be performed to check the performance for the proposed one. A description of the GPU implementation will be presented as well as some applications to tsunami simulation in real topo-bathymetries.

Recent trends in modeling, analysis, and simulation of induction heat treatments

Optimisation of crystal growth from the melt using magnetic fields: some mathematical aspects

Pierre-Etienne Druet

Author Keywords: Electromagnetic heat production, Low-frequency Maxwell equations, Analysis and optimal control of coupled systems of PDEs.

Abstract

In metallurgy magnetic fields are usually known for their stabilising properties on liquid metals subject to thermal convection: In particular in the context of semiconductor single crystal growth from the melt, these stabilising effects have raised recent attention. We refer about the project 'Numerical Simulation and Optimisation of Crystal Growth From the Melt Using Travelling Magnetic Fields' carried over in the context of the DFG research centre Matheon in Berlin. The magnetic field applied to influence the flow directly interacts with the heating system of the high temperatures furnace. We will start presenting a model that takes into account the melt flow, the global heat transfer and the applied magnetic fields in this application. For its more specialised part, the talk will focus on theoretical aspects of the analysis of the low-frequency Maxwell equations and of the optimisation problem. In particular, we will show the importance of the concept of vector fields satisfying divergence and rotation constraints in dual Sobolev spaces. Compact embedding results and regularity properties for such fields

allow to deal with the difficult coupling to the heat equation in the context of optimal control, also in the complex geometrical settings typical for industrial applications.

Modelling and Simulation of Multifrequency Induction Hardening for Gear Components

Thomas Petzold

Author Keywords: Induction hardening, Maxwell equations, Finite element method, Multi field problem.

Abstract

Induction hardening is a modern method for the heat treatment of steel components. Targeted heating of the surface layer by means of electromagnetic fields and subsequent quenching leads to surface hardening of the workpiece. For multifrequency induction hardening, currents with two frequencies (medium- and high-frequency) are fed simultaneously to a single induction coil to generate eddy currents in the part. For gears, this can lead to a hardness profile following the contour of the part. Because of the complex interrelationship, numerical simulations of the process gain increasing importance.

A model for the 3D simulation of multifrequency induction hardening of steel components is presented. It consists of a coupled, nonlinear system of partial differential equations for the determination of the electromagnetic fields, the temperature and the phase distribution in the workpiece.

Due to the skin effect and the occurrence of different time scales for the various physical processes, the model represents a nonlinear multi-scale

problem in space and time. The resulting equations are solved using adaptive finite element methods, Maxwell equations are discretized by edge elements. The consideration of non-linearities arising from temperature dependent material parameters as well as a magnetic permeability depending on the magnetic field itself is essential for the reproduction of experimental results.

The use of a non-commercial finite element solver allows for an efficient implementation in C/C++, which is adapted to the computer architecture and can take advantage of widely used multi-core processors. Furthermore, adaptive algorithms for grid generation lead to a reduction in the number of degrees of freedom and allow for an error control at the same time, leading to a gain in computational performance.

In addition to numerical simulations, experimental verifications for the surface hardening of discs and gears are presented. There is a good agreement between the experimental results and the calculated temperature and hardness profiles.

Modelling and Simulation of the Thermomechanics of Induction Heat Treatment

Alfred Schmidt, Qingzhe Liu, and Jonathan Montalvo Urquizo
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Abstract

Distortion and residual stresses are important aspects of any heat treatment. We present a thermomechanical model and simulation results for the heating and quenching during an induction heat treatment of rings and cogwheels. The model includes phase transitions and transformation induced plasticity (TRIP). FEM simulation results show the importance of including TRIP effects and a good agreement with experimental results for residual stresses after the heat treatment.

Simulations use the pdelib toolbox from WIAS Berlin.

This work was part of a collaboration project *MeFreSim* joint with WIAS Berlin, University of Augsburg, and IWT Bremen. We gratefully acknowledge the financial support of BMBF.

Analysis of potential Maxwell's equations in the harmonic regime with nonuniformly elliptic electric conductivity

M. T. González Montesinos and F. Ortegón Gallego [115]

Abstract

We analyze a nonlinear strongly coupled system of PDEs arising in the heating induction-conduction process of steel hardening. This model consists of the potential Maxwell equations in harmonic regime coupled with an energy balance equation. This leads to a system of elliptic-parabolic nonlinear equations, namely

$$-\nabla\cdot(\sigma(\theta)\nabla\varphi) = i\lambda\omega\nabla\cdot(\sigma(\theta)\mathbf{A}) - \nabla\cdot(\sigma(\theta)\nabla\varphi^0) \text{ in } \Omega_T, \tag{4}$$

$$\varphi = 0 \text{ on } \Gamma_0\times(0,T), \quad \frac{\partial\varphi}{\partial n} = i\lambda\omega\mathbf{A}\cdot n \text{ on } \Gamma_1\times(0,T), \tag{5}$$

$$i\omega\sigma(\theta)\mathbf{A} + \nabla\times(\frac{1}{\mu}\nabla\times\mathbf{A}) = -\sigma(\theta)\nabla\varphi \text{ in } D_T \tag{6}$$

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$$\nabla \cdot \mathbf{A} = 0 \text{ in } D_T, \quad \mathbf{A} \cdot n = 0 \text{ on } \partial D \times (0,T), \tag{7}$$

$$\rho c_e \frac{\partial \theta}{\partial t} - \nabla \cdot (\kappa(\theta) \nabla \theta) = \frac{\sigma(\theta)}{2} |i\omega \mathbf{A} + \nabla \varphi|^2 + G \text{ in } \Omega_T, \tag{8}$$

$$\frac{\partial \theta}{\partial n} = 0 \text{ on } \partial\Omega \times (0,T), \quad \theta(\cdot, 0) = \theta_0 \text{ in } \Omega, \tag{9}$$

where φ comes from the electric potential, $\mathbf{A}$ comes from the vector magnetic potential, and θ is the temperature. In this setting, we assume that the electric conductivity is nonuniformly elliptic which yields to a very complex situation.

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Simulation and control of hot-rolling

Optimal control approach for production of multiphase steels

Dietmar Hoemberg, Klaus Krumbiegel and Nataliya Togobytska

Author Keywords: optimal control, optimality conditions, hot rolling, dual phase steel.

Abstract

Multiphase steels combine good formability properties with high strength and have therefore become important construction materials, especially in automotive industry. The standard process route is hot rolling with subsequent controlled cooling to adjust the desired phase mixture. Here, the most important control parameters are the amount of water flowing per time 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 also in practice. The problem of the controlled cooling can be considered as an optimal control problem, where the state equations are a semilinear heat equation and an ordinary differential equation, which describes the evolution of the ferrite phase fraction. The optimal control problem is analyzed and the first-oder necessary and second-order sufficient optimality conditions are derived. 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 Mo-Mn dual phase steel.

Model reduction for rolling problems

Jens Seidel

Author Keywords: model reduction, POD, DEIM, finite element approximation, numerical simulation.

The Proper Orthogonal Decomposition (POD) model reduction approach is used to accelerate the simulation of a cold-rolling process which is strongly nonlinear. For dealing efficiently with the nonlinearities POD is combined with the Discrete Empirical Interpolation Method (DEIM).

In the industry often simplified models are used which ignore certain physical details such as shear stresses and lead to fast simulations suitable for online control. They are often based on a one-dimensional calculation using the Karman equation for stress development.

In contrast to such models the presented method uses a flow formulation and determines the coupled process parameters temperature, stress, strain and strain rate for the steady-state. The deformation power functional is minimized and consists of plastic deformations, friction between workpiece and roll as well as external forces. Elastic deformations are ignored in the model as they are small compared to plastic ones.

For the discretization of the model the Taylor-Hood finite element is used. To find the stationary point of the power functional as a function of the finite element degrees of freedom Newtons method is applied. This requires a regularization to ensure that the functional is differentiable.

In particular due to the nonlinear hardening law, solving the full discretized problem is not feasible in real time and the most time consuming part is the calculation of the strain. Restricting the problem to a lower dimensional subspace using POD allows for a much faster computation since a small subspace is sufficient to describe the model accurately for different

process parameters. This provides an alternative to the one-dimensional model which is both fast and accurate.

Nucleation, growth, and grain size evolution in dual phase steels

Dietmar Hoemberg, Shuai Lu and Masahiro Yamamoto

Author Keywords: nucleation and growth, dilatometer experiment, phase transition.

In this talk we review models suitable to describe the ferrite growth in dual phase steels. We revisit the classical Johnson-Mehl-Avrami-Kolmogorov nucleation and growth models and show how to use this approach to account also for soft impingement effects. We show how phase transition kinetics can be identified from dilatometer measurements and identify temperature dependent nucleation rates for generalised Avrami models.

Methods for Advanced Multi-Objective Optimization for eDFY of complex Nano-scale Circuits

Yield Optimization in Electronic Circuits Design

Vittorio Latorre, Gianni Di Pillo and Angelo Ciccazzo

Author Keywords: Yield Optimization, Derivative Free Optimization, Surrogate Models, Support Vector Machines.

Abstract

In electronic circuits production the yield is the percentage of circuits that satises all performance features, in dierent operating conditions and despite of random process variations. The yield optimization turns out to be the black box optimization of a function evaluated by expensive circuit simulations whose derivatives are not available. In the context of the MAnON European Research Program aiming at improving the production processes of the electronic industry, we propose an approach to yield optimization that combines the use of a Support Vector Machine as surrogate model of the circuit and of a Mixed-Integer Derivative Free optimization algorithm as black box optimization tool. As an example, we report the results obtained in the design of a DC-DC converter, compared with the results obtained using the commercial software currently adopted by ST-Microelectronic for this kind of applications.

Application of mathematical methods to the modeling and optimization of logic cell performance

Zia Abbas and Mauro Olivieri

The progressive downsizing of CMOS channel length lead to enormous increase in process variability and therefore degrading the Integrated Circuit (IC) fabrication outcome. However, technology scaling always done to fulfill the demand of semiconductor manufacturing industry for the higher number of transistor and therefore more number of functions in a single IC, greater performances i.e. less delays and high yield. This increased complexity and miniaturization of transistors put a challenge in IC design and manufacturing due to increased critical process variations. As a result, transistors behave and interact in a complex manner. Consequently, optimization for yield has become one of the crucial tasks in Integrated Circuit (IC) design.

The statistical variations whether global, local or otherwise have to be thoughtfully accounted, if we have to achieve low power, high-performance and high yield design goals. In the current scenario of IC design, specifications of many circuits have challenging trade-off and require multi-dimensional, multi-objective optimization, therefore needed enough insight into the optimization skill of the circuits. In this context, the role of techniques for circuit analysis and yield optimization became essential to obtain different solutions that satisfy the requested performance with the less time effort. Transistor level designs like standard cells are also most susceptible to parametric yield issues caused by process variations. The digital process corners are becoming ineffective as the design can be operational at all

corners but not at some combination of intermediate values.

Sizing and yield optimization of digital standard cells have been carried out for performance figures like *low to high*, *high to low* delays and pattern dependent leakages including 9 global process variations and 10 local i.e. mismatch variations for each device in circuit under worst case operating conditions. The operating variations like temperature and supply voltage have been specified in range of -40^{o}C to 125^{o}C and 0.95V to 1.05V respectively. The net lists of standard cells have been designed and simulated in HSPICE using 40nm CMOS Low Power standard threshold voltage (svt) process development kit (PDK) with statistical models.

In sizing and optimization process of the standard cells, the design parameters (length and width) of transistors have been changes in order to fulfill the given specification of the cells. Appropriate design parameter values have been calculated such that the performances are optimal under the influence of statistical variations and must be functional as long as in the range of operating variations. The sizing and optimization have been divided in nominal optimization under worst-case operating condition (without the influence of process variations) and yield optimization under worst case operating condition (with the influence of process variations). Later Monte Carlo analysis has also been performed to verify the robustness i.e. estimated yield of the standard cells.

On the other hand, generation of reliable model (like Response Surface Model) with reduction in the effort, ensuring model accuracy as high as possible is also one of the challenging tasks especially for present high statistical variations due to technology scaling. The RSM model generations of standard cells have also been carried out for delays and leakage performance including statistical variations from 40nm LP svt PDK. The generated model also compare with other models like ANN and SVM.

The usage of Symbolic Model Order Reduction techniques for reducing the complexity of a system of differential-algebraic equations describing the behaviour of an integrated circuit, thus reducing drastically the simulation time

Patrick Lang, Matthias Hauser and Mohammed Ali Khozoei

Author Keywords: Analog Insydes, Symbolic Model, Symbolic Model Order Reduction, Fraunhofer.

Abstract

We present the last version of our software Analog Insydes, a Mathematica toolbox for modelling, analysis, and design of analogue systems, tailored specifically for industrial applications.

We present recent advances in the mixed symbolic and numeric model reduction techniques for automatically extracting the dominant system behaviour of metaphysical systems. A unique feature of our approach is to compute approximated symbolic formulas for linear and nonlinear system characteristics, rigorously reducing the complexity of symbolic expressions while controlling a user given error bound. Yielding a symbolic description in terms of crucial design parameters we handle problems not using purely numeric methods. We improved our established methods for analyzing industrial-sized systems and extended insights into their behaviour.

Furthermore, an overview of the newest enhancements will be given that enables the usage of Analog Insydes capabilities in extended fields of application.

A Wicked based framework for circuit modelling and statistical circuit optimization

Mohammed Ali Khozoei and Carmelo Vicari [116]

Abstract

In the field of Integrated Circuit (IC) design the continuous reduction of device dimensions makes circuit performances such as power dissipation and delay more and more sensitive to the inevitable fluctuation of process parameters. In order to avoid significant yield loss the impact of statistical variations in the production processes must be taken into account already in design phase. This is done by estimating the statistical distribution of the circuit performances that are influenced by the random variation of process parameters. These distributions are then used to fine tune the design parameters such that the portion of manufactured devices that meet the specifications is maximized under all operating conditions. One method to statistically characterize circuit performances is using computationally expensive Monte Carlo methods. The number of SPICE simulations needed to perform a Monte Carlo analysis can be reduced by creating mathemat-

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ical models which approximate the performances of interest of a circuit as function of the statistical parameters. In general this relationship is not known analytically and can be obtained only via computer simulations. In these cases Response Surface Methodology (RSM) and Machine Learning techniques, such as Artificial Neural Networks (ANN) and Support Vector Machines (SVM), are promising approaches for building performance models from a reduced number of SPICE simulations. If the accuracy of these models is adequate, they can then be used to execute large run Monte Carlo simulations thus reducing considerably the time needed for statistical circuit optimization. The generation of such kind of models is not trivial. Usually one has to test different modelling approaches to find the one that performs better in terms of accuracy and computational effort. Often, to simplify the learning process, preliminary analyses such as parameter screening or mathematical transformation of input/output parameters are necessary. Additionally, a fine tuning of a set of model parameters is important to avoid phenomena such as overfitting or underfitting. We present a software framework which simplifies and automatizes the generation of performance models. These models are used in combination with a line search derivative free optimization algorithm for the yield optimization of digital and analog electronic circuits. The framework is written in Python and based on WiCkeD, a widely used EDA software tool for circuit analysis, modeling and optimization. WiCkeD provides a scripting module which allows to easily interact with any kind of circuits and PDKs and contains a module for the generation of RSM models. The framework lets the user to use two additional methodologies, ANN and SVM, for the estimation of circuit performances. The method performing better in terms of accuracy and computational effort is automatically chosen. To improve the accuracy, the framework allows the generation of a set of local models, each valid in a subset of the parameter space or for fixed values of design and operating parameters. It includes algorithms for sampling the parameter space to generate training and test sets, model error checking and regularization methods.

The usage of neural networks to reduce simulation time of transient analysis

Mohammed Ali Khozoei and Angelo Ciccazzo

Author Keywords: simulation, Model, neural network, approximation.

Abstract

The production of semiconductor integrated circuits is very complex and expensive. Therefore it is essential to verify the designed circuits before their production.

In general the values of some circuit variables, called circuit outputs, describe the performances of the circuit and have to satisfy the related specifications. One way to verify that designed circuit satisfies its specifications is the simulation of its behaviour. But the SPICE simulation of a complex systems can be very time consuming and consequently expensive.

Usually a circuit has to be simulated many times during the design flow, for example to find the optimal values of some design parameters or optimizing the yield. In such situations the values of a set of circuit parameters will be changed and the specifications of the output variables will be verified. Due to the complexity of such circuits and the high number of simulations, such analyses are very expensive. For this reason the industry is deeply interested in using less complex but accurate models to replace time consuming SPICE simulations.

On the one hand, very often wave form of the circuit outputs do not significantly change by such analyses. A model which estimates these functions

can replace the simulation of the circuit for computing the performances and so the number of the circuit simulations will be extremely reduced. On the other hand, the circuit can contain sub circuits with the output signals which hardly change by different values of the parameters under test. In this case, these sub circuits can be replaced by some models which estimate these signals and so the complexity of the system will be extremely reduced.

Based on these facts, this contribution presents a method that can be used either to reduce the number of simulations of an electronic circuit or to create compact models that can replace sub circuits of a very complex system.

The models generated by this method approximate the functions of the output variables by using Bézier curves independently of the complexity of the circuit.

This contribution will present the usage of neural networks to determine these Bézier curves for different parameter values.

This method has been implemented and tested in the industrial environment supported by STMicroelectonics.

Derivative-free methods for multiobjective Lipschitz problems

Stefano Lucidi, Gianni Fasano, Giampaolo Liuzzi and Francesco Rinaldi

Author Keywords: Optimization methods, Non linear constrained multiobjective problems, Derivative free methods

Abstract

The optimal design of complex devices often presents the following difficulties:

- it involves many variables which nonlinearly affects all the features of the device;
- it needs the variables to be chosen in such a way that the design is feasible;
- it involves various conflicting objectives and goals.

These problems can be modeled as nonlinear constrained multiobjective optimization problems in which

the first order derivatives of the objective function and constraints can be neither calculated nor approximated. In this work we propose derivative-free methods for solving the previous class of problems First we show the equivalence between the original constrained multiobjective problem, and a multiobjective problem with simple bounds, by means of an exact penalty function approach. Then we propose a line search based derivative free framework for the problem with simple bounds and report some numerical results proving the effectiveness of the proposed approach.

Models of drift-diffusion for concentrated solutions

A new continuum mixture theory of electrolytic solutions containing solvation effects

Manuel Landstorfer, Clemens Guhlke and Wolfgang Dreyer

Author keywords: Poisson-Boltzmann Gouy-Chapman-Stern Double Layer Metal/Electrolyte Interface Solvation

Abstract

In this talk a new continuum mechanical mixture theory of a liquid solution containing dissociated ions is presented. It explicitly incorporates solvation effects in the entropy of mixing as well as in the mechanical contribution of the free energy, which leads to new chemical potentials for all constituents. With this it is shown that in the thermodynamic equilibrium the free charge density in the electrolyte is inherently a function of pressure and the electrostatic potential, which is in contrast to almost all classical modelling approaches (eg. Gouy-Chapman, Poisson-Boltzmann, Bikerman, ...). In consequence, the Poisson equation and the momentum balance do not decouple (even in equilibrium), which should be considered as the generic case of electrolytic solutions. A comparison of the new model to the Gouy-Chapman, Poisson-Boltzmann and the ideal, incompressible mixture model will be given during the talk, which unequivocally shows the shortcomings of these classical approaches. The computed capacity of the metal/electrolyte interface for various salt concentrations is, for the first time, in remarkable quantitative and qualitative agreement with single crystal experimen-

tal data. The model thus reveals some unimagined predictive strength of continuum thermodynamics in electrochemistry and could be considered as basis for non-equilibrium drift-diffusion equations of electrolytic solutions.

Nonlinear Poisson-Nernst-Planck Equations for ion flux through confined geometries

Martin Burger, Baerbel Schlake and Marie-Therese Wolfram

Author Keywords: Nonlinear Poisson-Nernst-Planck equations, Size exclusion, Cross diffusion, Numerical simulations

The mathematical modeling and simulation of ion transport trough biological and synthetic channels is a challenging problem, with direct application in biophysics, physiology and chemistry. At least two major effects have to be taken into account when creating such models: the electrostatic interaction of ions and the effects due to size exclusion in narrow regions. Recently several papers proposed simple or sophisticated approaches for including size exclusion effects into entropies, in equilibrium as well as off equilibrium. In this talk we present a potentially important modification due to size exclusion, namely the modification of mobilities due to size exclusion effects. We discuss a simple model derived from a self-consisted random walk and investigate the stationary solutions as well as the computation of conductance. The need of incorporating nonlinear mobilities in high density situations is demonstrated in an investigation of conductance as a function of bath concentrations, which does not lead to obvious saturation effects in the case of linear mobility.

Excluded volume effects in drift diffusion

Jon Chapman and Maria Bruna

Author Keywords: matched asymptotic expansions, diffusion, Fokker-Planck equation, excluded volume, Poisson-Nernst-Planck equation, Poisson-Boltzmann equation.

Abstract

When diffusing agents interact with each other their motions are correlated, and the configuration space is of very high dimension. Often an equation for the marginal distribution function of one particle (the "concentration") is sought by "integrating out" the positions of all the others. This leads to the classic problem of closure, since the equation for the concentration so derived depends on the two-point correlation function. A common closure is to assume independence at this stage, leading to some form of nonlinear (drift) diffusion equation. Such an approach works well for long range interactions (such as electric fields), but fails for short range interactions (such as steric effects).

Here we consider an alternative approach using matched asymptotic expansions, in which the approximation is entirely systematic, and in which both long and short range forces can be incorporated.

Physics-based modelling of lithium-ion batteries using orthogonal collocation

A.M. Bizeray, S.R. Duncan and D.A. Howey[117]

Abstract

We discuss the numerical solution using orthogonal collocation of a physics-based lithium-ion battery model, the so called Newman model or pseudo-two dimensional (P2D) model. We aim at reducing the computational cost of the solution of the P2D model compared to using the finite difference method without losing the physical meaning of the model parameters. The goal is to solve such a physics-based model combined to a state observer online an electric vehicles battery management system (BMS) to provide accurate battery state estimation - state-of-charge (SOC), power capability and state-of-health (SOH). Currently, BMSs use relatively simple system dynamics models, such as empirical equivalent electrical circuits, for on-line battery state estimation due to their low computational requirements. However, these are valid for a narrow range of operating conditions and have little physical meaning. In particular, such empirical models are usually only

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valid at low currents and accounting for battery degradation is difficult. The physics-based P2D model, which is based on the porous electrode theory and the concentrated solution theory, consists of conservation equations governing species concentration and electrostatic potential. By accounting for the diffusion of lithium with possibly concentration-dependent transport properties, the P2D model can accurately describe the battery behaviour during high current operation. Furthermore, by virtue of its physical meaning, the P2D model can include temperature and battery ageing effects directly. Physics-based models been widely used for battery design, but are computationally intensive and therefore are not implemented in embedded systems for real-time battery management. We present a computationally efficient solution of the P2D model using orthogonal collocation that could be used within a BMS. We have implemented the orthogonal collocation numerical method instead of the commonly used finite difference method to solve the differential-algebraic equations (DAEs) system of the P2D model. This results in a much lower order system of equations that maintains the accuracy even at high C-rates (40C). The model is implemented using a control engineering state-space approach solved in Matlab. We also used our implementation of the P2D model to design an extended Kalman filter for state estimation that may be used within an embedded processor for real-time on-board application.

Mathematical Modelling of Photovoltaic Devices

Understanding Photoluminescent properties of Organolead Halide Perovskite

Victor Burlakov, Samuel Stranks, Tomas Leijtens, James Ball, Henry Snaith and Alain Goriely

Author Keywords: Photoluminescence, Organolead Halide Perovskite, Electronic traps, Excitons

Abstract

Organic-inorganic perovskites have been attracting an enormous amount of recent attention for their use in high-performance solar cells. Using photoluminescence data obtained under pulsed and continuous excitations for the perovskite CH3NH3PbI$(3-x)$Cl(x) we have developed a model describing the evolution of photo-excited charges in the presence of electronic mid-gap trap states. The model parameters governing kinetics of free charge carriers, excitons and electronic traps in this material indicate that photoluminescence is due to excitons, which either dissociate producing free electrons and holes, or decay radiatively. In contrast, the photoexcited free electrons may fill the traps, form excitons or recombine non-radiatively with holes. The model description of the photoluminescence at different temperatures strongly indicates that the trap concentration increases with temperature suggesting an intrinsic origin of trap states. Our results provide an understanding of how to optimize the material performance for high-performance solar cells and high efficiency light emitting diodes.

Controlled topological transformations in a binary mixture confined to a thin-film geometry

Matthew Hennessy, Victor Burlakov, Andreas Münch, Barbara Wagner and Alain Goriely

In this talk we consider the dynamics of a binary mixture that is confined between two walls of infinite horizontal extent. The evolution of the mixture is described by a diffusive phase-field model and we assume that the constituent phases, A and B, are preferentially attracted to oppo- site walls. When the temperature of the system is slowly lowered below the bulk critical point, we find that the bias of the walls causes the mixture to separate into a bilayer configuration. The two layers are separated by a thin interfacial region where the composition changes rapidly. This bilayer *interface* runs parallel to the walls and its long length suggests that the bilayer does not correspond to the state of lowest energy. We show that a local perturbation to the bilayer interface can trigger the onset of a self-sustaining sequence of ruptures that transforms the bilayer into a repeating series of laterally-separated alternating A-rich and B-rich domains. The formation of regular structures in thin-film geometries is likely to be of particular interest to researchers working with composite materials to produce organic solar cells and other nano- devices. The dynamics of the transformation are investigated by reducing the phase-field model to a sharp-interface model which can be further simplified to a thin-film equation.

Mathematical modelling of contact resistance in silicon photovoltaic cells

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Abstract

In screen-printed silicon-crystalline solar cells, the contact resistance of a thin interfacial glass layer of varying thickness (10 nm - 1m) between the silicon and silver electrode inhibits electron ow and degrades the solar cell performance. In this paper we analyse a model for electron transport across the glass based on the 2D drift-diffusion equations. The mathematical model consists of a system of coupled non- linear elliptic partial differential equations for the electric potential and the electron density. We use complex variable techniques to map the equations to a rectangle, and solve the resulting mapped problem numerically using a new 2D spectral method. As well as the predicted resistance of the glass layer, we are able to determine the trajectories of the electrons through and the degree to which the current *short-circuits* through thin regions. The numerical results are compared with asymptotic predictions obtained in limiting cases.

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Two-phase flow model for suspensions with yield-stress behavior

Tobias Ahnert and Andreas Münch and Barbara Wagner[119]

Abstract

In order to model the drying behavior of an organic solar cell, we propose a two-phase model based on ensemble averaging. We use constitutive laws producing an yield-stress behavior. For simple channel flow we can show a reduction of the system to a free boundary ODE system that can be studied using phase space methods. In the talk a discussion of the model will be given.

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Bayesian and approximative sampling methods for Uncertainty Quantification

Parameter estimation in large scale state space models using ensembles of model runs

Marko Laine and Heikki Haario

Author Keywords: numerical weather prediction, parameter estimation, uncertainty quantification, ensemble methods

Abstract

Estimation of static model parameters is an important topic in tuning of large scale dynamical models, such as those for atmosphere, weather or oceans. These multi-scale models contain so called closure parameters that are needed in parameterizations of unresolved sub-grid scale processes. The parameters are considered as static, but there is an inherit uncertainty coming from the model discrepancy, causing the optimal parameter value to depend on the current model state. A conceptually simple hierarchical statistical description of this forward model uncertainty is presented. It allows the estimation of static parameters and their uncertainty from the between model ensemble variability. The estimation technique is targeted to solve the problem of closure parameter tuning in large scale operational models in numerical weather prediction. For those models, existing assimilation systems and model ensemble prediction systems are already available. By adding parameter perturbations to the ensemble systems, we gain information on the parameter uncertainty. This method has been implemented and tested in European Centre for Medium-Range Weather Forecasts (ECMWF) in their numerical weather prediction (NWP) model.

Reference

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Tuning parameters of Ensemble Prediction System and optimization with Differential Evolution approach

Vladimir Shemyakin and Heikki Haario [120]

Abstract

Ensemble Prediction System (EPS) is the approach used in present day weather predictions to estimate the uncertainty of predictions. Along with the main prediction an ensemble of simulations is launched with perturbed initial values. Recently, the EPS with simultaneous parameter estimation approach (EPPES) has been proposed to tune model parameters online, without additional computational costs, by perturbing the parameter values and monitoring the respective performances. The key point of EPPES is the estimation of parameter covariance by sequentially updating the covariance as hyperparameters by aid of importance weights. A problem, however, is the choice and weighting of cost functions, as several criteria should be simultaneously satisfied.

Here, we present an approach to automatically scale various criteria together by a method of separate EPPES importance weights. Moreover, we

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study the Differential Evolution (DE) optimization approach to solve the problem as a stochastic optimization task. We show that the convergence is improved using DE, in case the initial values of model parameters are far enough from the true ones.

Stabilizing correction for approximative low-memory Kalman filtering. Extensions and generalizations

Alexander Bibov and Heikki Haario

Author Keywords: data assimilation, parallel data assimilation, approximate Kalman filter, L-BFGS, chaotic dynamics, parallel filtering.

The Kalman filter is a known statistical tool used for optimal estimation of dynamical system states. The estimation is performed by combining information from model that describes time evolution of the system and from external observations. Layout of the Kalman filter is best described by predictor-corrector scheme. A filter iteration gets initialized by a known starting point (usually derived from the previous step of the filter), which is then extrapolated forward over the time by transition model. The rest of the iteration is a correcting procedure that compares prediction with observed data and introduces appropriate corrections.

Classical Kalman filter is limited by requirement of linearity applied to prediction model. This assumption can be relaxed by leveraging common linearization approaches, which leads to the extended Kalman filter (EKF). However, while dimension of the state space increases, both classical and extended formulations become inefficient due to impracticably large covariance matrices of the estimates. In the previous studies it was proposed to replace the problematic matrices by their low-memory approximations generated using L-BFGS optimization algorithm. This idea allows to implement L-BFGS EKF, which however does not guarantee nonnegative-definiteness of the approximate state estimate covariance matrices. In the present work

we suggest a way to alleviate this problem by introducing a family of stabilizing corrections. We prove that when these corrections are used, the approximated covariance matrices remain nonnegative-definite. Moreover, we demonstrate that our modification ensures quadratic convergence of the approximate filter towards the EKF, whereas the previously suggested L-BFGS EKF guarantees only linear rate of convergence.

In order to assess estimation performance of the approximate Kalman filters, we employ two-layer Quasi-Geostrophic model as a benchmark case . The model is chaotic, cheap to run and can be made large-scale by adjusting density of its spatial discretization grid. We demonstrate that L-BFGS EKF develops unstable behavior when dimension of the state space becomes sufficiently large. Opposite to this, the "corrected" version, which uses our stabilizing correction, performs equally well in all of our experiments regardless of the state space dimension.

Finally, we discuss further extension of the stabilized approximate Kalman filter to the case of parallel filtering, where several states get propagated at once during single prediction step. We describe relations between this approach and the weak-constraint 4D-VAR (an emerging method for parallel data assimilation) and provide results of experimental comparison between the parallel filter, the weak-constraint 4D-VAR and the single state stabilized approximate Kalman filter.

Natures natural order: from individual to collective behaviour and self-organization

Mathematical and numerical analysis of a coupled anisotropic chemotaxis-fluid model

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Keywords

Chemotaxis, Anisotropy, Degenerate Parabolic Equation, Finite Volume, Finite Element, Navier-Stokes equations.

In this paper, we consider a chemotaxis-fluid model arising from biology, consisting of parabolic-parabolic chemotaxis equations coupled to viscous incompressible Navier-Stokes equations by transport and gravitational forcing. The motivation of this model is the study of the behavior of many cell organisms towards a chemo-attractant in a fluid. For example, bacteria often swim towards higher concentration of oxygen to survive. The unknowns are the density of cells, the concentration of chemo-attractant, the velocity and the pressure in the fluid. In space dimensions less or equal than three, we first proved global existence of weak solutions for the chemotaxis-Navier-

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Stokes system in [1]. When the fluid is at rest, a finite volume scheme has been studied in [2] to discretize the isotropic chemotaxis model. However, standard finite volume scheme not permit to handle anisotropic diffusion on general meshes and it is well-known that finite element discretization does not impose any restrictions on the meshes but many numerical instabilities may arise in the convection dominated case. Therefore, a combined finite volume-nonconforming finite element method scheme has been recently developed in [3] to discretize the anisotropic chemotaxis model. In the case of non positive transmissibilities, the discrete maximum principle is no more guaranteed. For that, the authors in [3] elaborate in the spirit of methods described in [5], a general approach to construct a nonlinear correction providing a discrete maximum principle while retaining the main properties of the scheme, in particular coercivity and convergence toward the weak solution of the continuous problem.

Taking into consideration the discretization of the Navier-Stokes equations by nonconforming finite element method in [4], our aim now is to extend the idea of the monotone combined scheme to the anisotropic chemotaxis-fluid model. Many numerical tests will be given to improve the effectiveness of this numerical scheme.

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Mechanoregulation of molecular motors in flagella

Hermes Gadelha

Author Keywords: Molecular motors, flagella, self-oscillation, cell swimming.

Abstract

Molecular motors are nano-biological machines responsible for exerting forces that drive movement in living organisms, from cargo transport to cell division and motility. Interestingly, despite the inherent complexity of many interacting motors, order and structure may arise naturally, as exemplified by the harmonic, self-organized undulatory motion of the flagellum. The real mechanisms behind this collective spontaneous oscillation are still unknown, and it is challenging task to measure experimentally the molecular motor dynamics within the flagellar structure in real time. In this talk we will explore different competing hypotheses that are capable of generating flagellar bending waves that resemble in-vitro observations, emphasizing the need for further mathematical analysis and model validation. It also highlights that this is a fertile and challenging area of inter-disciplinary research for applied mathematicians and demonstrates the importance of future observational and theoretical studies in understanding the underlying mechanics of these motile cell appendages.

Flagellar synchronisation through direct hydrodynamic interactions

Marco Polin, Douglas Brumley, Kirsty Y. Wan and Raymond E. Goldstein

Author Keywords: Flagella, Synchronisation, Biological oscillator, Microhydrodynamic, Biological noise.

Abstract

Microscale fluid flows generated by ensembles of beating eukaryotic flagella are crucial to fundamental processes such as development, motility and sensing. Despite significant experimental and theoretical progress, the underlying physical mechanisms behind this striking coordination remain unclear. Here, we present a novel series of experiments in which the flagellar dynamics of two micropipette-held somatic cells of Volvox carteri, with measurably different intrinsic beating frequencies, are studied by high-speed imaging as a function of their mutual separation and orientation. From analysis of beating time series we find that the interflagellar coupling, which is constrained by the lack of chemical and mechanical connections between the cells to be purely hydrodynamical, exhibits a spatial dependence that is consistent with theoretical predictions. At close spacings it produces robust synchrony which can prevail for thousands of flagellar beats, while at increasing separations this synchrony is systematically degraded by stochastic processes. Manipulation of the relative flagellar orientation reveals the existence of both in-phase and antiphase synchronized states, which is consistent with dynamical theories. Through dynamic flagellar tracking with exquisite spatio-temporal precision, we quantify changes in beating waveforms that

result from altered coupling configuration and distance of separation. The experimental results of this study prove unequivocally that flagella coupled solely through a fluid medium can achieve robust synchrony despite significant differences in their intrinsic properties.

Stochastic multi-scale modelling of filopodial growth

Ulrich Dobramysl and Radek Erban[122]

Abstract

Many types of migrating cells display membrane protrusions, so-called filopodia. These cytoplasmic projections contribute to environmental sensing and chemotaxis, cell motility, establishment of mechanical cell connections during wound healing, neural growth, and other functions. They consist of a highlyorganized set of bundled actin filaments that are rooted in the cytoskeleton. Polymerization of actin at filament tips is influenced by various proteins such as formins and capping proteins and competes with depolymerization at the filopodial root (retraction). Thus, filopodia have a limited lifetime. Here, we present a three-dimensional model for filopodial growth and collapse. We simulate protein dynamics using an adaptive hybrid multiscale algorithm, wherein proteins in the vicinity of filament tips are modeled by employing an off-lattice Brownian dynamics method. An efficient compartment-based algorithm is used in the remainder of the computational domain to correctly capture the diffusive spread of proteins. Using this technique, we study the influence of diffusive noise on the lifetime of filopodia.

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Model Based Optimization of Industrial Processes

Microbial Enhanced Oil Recovery and efficient Parameter Estimation

Robert Kircheis, Stefan Körkel and Michael Rieger

Author Keywords: enhanced oil recovery, parameter estimation, model validation.

Abstract

Microbial Enhanced Oil Recovery (MEOR) is a so called tertiary oil extraction technology allowing the partial recovery of oil entrapped in porous media, thus increasing the life time of mature oil reservoirs. When certain types of microbes are stimulated, i.e. supplied with nutrient, in core samples of reservoir sandstone in the laboratory, they improve oil production by mobilizing residual oil trapped in the pore space. The bacterial growth at an oil water interface causes a substantial reduction in interfacial tension and influences other parameters as porosity and permeability. Modeling this process is a challenging task. The model equations are of convection-diffusion-reaction type and have nonlinear dependencies on a set of parameter. The validation of the model is cooperation project among BASF and IWR Heidelberg. Therefor, we have developed an efficient parameter estimation algorithm based on a reduced approach to solve large scale problems. It allows multiple shooting structure exploitation with the effort of single shooting. BASF will provide the experimental data. Finally, we will show simulation runs of a 2D implementation of the model and results of the parameter estimation.

Model-based Optimization of Chemical Processes

Dr. Simeon Sauer, Dr. Robert M. Lee, Dr. Alexander Badinski
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Chemical process engineering is a prototypical application field for model-based optimization. Based on thermodynamic principles, it is possible to derive a mathematical process model that does not only fit the available experimental data sets, but is also predictive in operating windows that were not explored experimentally.

Chemical process engineering is a prototypical application field for model-based optimization. Based on thermodynamic principles, it is possible to derive a mathematical process model that does not only fit the available experimental data sets, but is also predictive in operating windows that were not explored experimentally.

Having found an accurate and validated process model, optimal control methods can then be applied to minimize the cost function of the process, e.g. by varying the temperature during the reaction or the inflow rate of the educts.

In this talk, we outline how chemists, physicists and mathematicians at BASF Ludwigshafen and at the IWR Heidelberg jointly work together to a) derive suitable process models for chemical reactors, b) minimize parameter uncertainties in the model through optimum experimental design, and c) use the resulting models to optimize the process.

In particular, we discuss how the software package VPLAN is used to estimate model parameters and to reduce their uncertainties through optimum experimental design. We illustrate the modeling workflow along examples from recent projects.

A Virtual Laboratory for Nonlinear Processes

Stefan Körkel

Author Keywords: differential equation models, model validation, model based optimization, software tool, industrial applications.

Industrial processes can often be described by nonlinear differential equation models. Usual model based tasks are simulation of the process states, sensitivity analysis wrt. certain input quantities, model validation by parameter estimation fitting experimental data and optimum experimental design computing the most significant experiments, and finally - using validated models - optimal design and optimal control of the processes.

These tasks require the solution of challenging initial and boundary value problems and nonlinear optimization and optimal control problems. We are developing tailored numerical methods for the differential equation constrained optimization problems of parameter estimation, optimum experimental design and optimal control based on direct multiple shooting, Newton-type optimization methods, adaptive error-controlled integration schemes, and automated derivative evaluation.

These methods are being implemented in our software VPLAN which provides a general purpose tool for ordinary differential algebraic equation models and a framework for the treatment of partial differential equation models.

In this talk, we present the application of our methods and software to case studies treated in collaboration with our industrial partners.

Efficient Calibration of Industrial Robots

Felix Jost, Stefan Körkel and Manuel Kudruss

Author Keywords: kinematic chain, optimum experimental design, collision constraints.

The calibration of industrial robots is an important task for their precise operation wrt. accuracy and repeatability.

We describe robots as kinematic chains using homogeneous transformations in Denavit-Hartenberg and Hayati formulation for the particular joints. Due to varying ambient conditions, the physical properties of the joints and thus the parameters of the homogeneous transformations may deviate from their reference values and have to be estimated from series of measurement data from different positions of the robot.

We collaborate with an industrial partner which provides an efficient measurement technology for this purpose.

The quality of the fit, i.e. the accuracy of the estimated parameters and thus the precision of the tool center point depends on the statistical uncertainty of the parameter estimate which can be described by its variance-covariance matrix. This depends on the positions of the robot during the experiments.

We apply methods of optimum experimental design in order to compute experimental series of positions which yield the most significant parameter estimate at given experiment effort and costs.

An important issue is the avoidance of collisions of parts of the robots with each other and with objects in the surroundings. This results in numerous nonlinear constraints which have to be satisfied in the optimization problem.

We formulate and solve these challenging nonlinear optimum experimen-

tal design problems with our software package VPLAN.

We present results from our industrial collaboration where the number of measurements to calibrate a robot has been reduced drastically by application of optimum experimental design.

Higher order models in mechanics, and numerical developments: non local and micromorphic materials, polar structural models and applications

A model of structural reorganisation in statistically oriented fibre-reinforced biological materials

Alfio Grillo, Raphael Prohl, Gabriel Wittum, Salvatore Federico[123]

Key words: Structural reorganisation, Fibre-reinforcement, Statistical composite materials

We present a mathematical model that describes the structural reorganisation of a fibre-reinforced composite material in which the fibres are oriented statistically according to a given probability density distribution. Under suitable working hypotheses, a composite material of this type may be thought of as an exemplification of a biological tissue, such as articular cartilage or a blood vessel.

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We assume that the structural reorganisation of the considered composite material, which is often referred to as *remodelling* in the biomechanical literature, manifests itself through the reorientation of the reinforcing fibres and the rearrangement (and/or development) of material inhomogeneities [2]. The former process concerns the evolution of the fibre pattern in the composite material; the latter one, instead, is related to the onset of inelastic deformations. Although these two processes are conceptually independent on one another, and may be governed by different characteristic time and length scales, they both lead to a variation of the internal structure of the material and may turn out to be intermingled.

We describe the reorientation of fibres by introducing a probability density distribution (PDD) that measures, for the composite material under investigation, the probability density of finding a family of fibres aligned along an assigned direction of space at a fixed material point [1].We hypothesise that the considered composite material is hyperelastic with respect to some relaxed state, and exhibits transverse isotropy with respect to a given symmetry axis. The latter condition places restrictions on the PDD. Moreover, we assume the PDD to be a Gaussian-like distribution, and denote by Q the angle that, at a given material point, the most probable direction of the local fibre alignment forms with the symmetry axis. We let the angle Q vary in time and space according to a self-consistently determined evolution law. Within this approach, we identify the time evolution of the angle Q as a measure of the structural reorganisation of the composite. This evolution, indeed, renders the PDD variable with time, while preserving its functional form. In our contribution, we summarise the results of this approach and discuss both its advantages and limitations.

With respect to the results reported in [1], the novelty of this contribution is twofold. Firstly, we couple the reorientation of fibres, modelled as described above, with the rearrangement of material inhomogeneities. In order to do this, we determine an evolution law for the tensor of inelastic deformations, which are assumed to depend on the stress state and the structure tensor, and discuss how the variation of the fibre pattern influences the rate of inelastic deformations both directly (by modulating the PDD) and indirectly (by changing the stress state). Secondly, we extend our framework to multiphasic materials. Finally, we briefly discuss a higher order constitutive description [3], in which also the gradient of the inelastic deformation tensor is accounted for.

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Network processes and differential equations

Controlling epidemic propagation on a network

Peter L Simon

Author keywords: Optimal Control, Proper Orthogonal Decomposition, Hamilton-Jacobi equations, Navier-Stokes equations

Abstract

We consider the approximation of an infinite horizon optimal control problem for an evolutive partial differential equation. The method is based on a model reduction technique, using a POD approximation, coupled with a Hamilton-Jacobi equation which characterizes the value function of the corresponding control problem for the reduced system. Although the approximation schemes available for the HJB are shown to be convergent for any dimension, in practice we need to restrict the dimension to rather low number (typically 4) and this limitation affects the accuracy of the POD approximation. We will present numerical tests for the control of the time-dependent Navier-Stokes system with two-dimensional spatial domains to illustrate our approach and to show the effectiveness of the method.

On a spatial epidemic propagation model

István Faragó and Róbert Horváth

Author keywords: numerical analysis, networks, partial differential equation, epidemic propagation

Abstract

Most of the models of epidemic propagation do not take into the account the spatial distribution of the individuals. They give only the temporal change of the number of the infected, susceptible and recovered patients. In our presentation we present a spatial epidemic propagation model and give some of its properties: the condition of forming epidemic waves, the speed of these waves, the behaviour of the model depending on the used parameters, etc. The results are demonstrated on numerical tests.

Exact deterministic representation of Markovian SIR epidemics on networks with and without loops

Istvan Kiss, Charles Morris, Fanni Selley, Peter Simon and Robert Wilkinson

Author Keywords: Master equation, Network, Closure, Loop, Cut-vertex.

In a previous paper Sharkey et al. (Bull Math Biol doi: 10.1007/s11538-013-9923-5, 2012) proved the exactness of closures at the level of triples for Markovian SIR (susceptible-infected-removed) dynamics on tree-like networks. This resulted in a deterministic representation of the epidemic dynamics on the network that can be numerically evaluated. In this paper, we extend this modelling framework to certain classes of networks exhibiting loops. We show that closures where the loops are kept intact are exact, and lead to a simplified and numerically solvable system of ODEs (ordinary-differential-equations). The findings of the paper lead us to a generalisation of closures that are based on partitioning the network around nodes that are cut-vertices (i.e. the removal of such a node leads to the network breaking down into at least two disjointed components or subnetworks). Exploiting this structural property of the network yields some natural closures, where the evolution of a particular state can typically be exactly given in terms of the corresponding or projected states on the subnetworks and the cut-vertex. A byproduct of this analysis is an alternative probabilistic proof of the exactness of the closures for tree-like networks presented in Sharkey et al. (Bull Math Biol doi:10.1007/s11538-013-9923-5, 2012). In this paper

we also elaborate on how the main result can be applied to more realistic networks, for which we write down the ODEs explicitly and compare output from these to results from simulation. Furthermore, we give a general, recipe-like method of how to apply the reduction by closures technique for arbitrary networks, and give an upper bound on the maximum number of equations needed for an exact representation.

PDE approximation of large systems of differential equations

Andras Batkai

Author Keywords: dynamical systems on networks, finite differences, large systems of ODEs.

A large system of ordinary differential equations is approximated by a parabolic partial differential equation with dynamic boundary condition and a different one with Robin boundary condition. Using the theory of differential operators with Wentzell boundary conditions and similar theories, we give estimates on the order of approximation. The theory is demonstrated on a voter model where the Fourier method applied to the PDE is of great advantage.

Differential equations from branching process models of popularity

James Gleeson

Author Keywords: networks, branching processes, complex systems.

Random-choice-with-innovation models offer a simplistic, yet sometimes surprisingly accurate, viewpoint on how consumers choose among multiple possible alternatives: e.g., what app to download, what YouTube video to watch, or what hashtag to use when tweeting? In this talk I review the mathematical basis of relevant branching processes models, with particular reference to our recent work on the popularity of memes on Twitter [Phys. Rev. Letters 112, 048701 (2014)], and extensions thereof.

Numerical methods for stiff problems in partial differential equations and applications

HIGH ORDER SEMI-IMPLICIT SCHEMES FOR TIME DEPENDENT PARTIAL DIFFERENTIAL EQUATIONS

Francis Filbet, Boscarino Sebastiano and Giovanni Russo

Author keywords: IMEX scheme, PDE, time discretization

Abstract

We consider a new formulation of implicit-explicit (IMEX) methods for the numerical discretization of time dependent partial differential equations. We construct several semi- implicit Runge-Kutta methods up to order three. This method is particularly well suited for problems where the stiff and non-stiff components cannot be well separated. We present different numerical simulations for reaction-diffusion, convection diffusion and nonlinear diffusion system of equations. Finally, we conclude by a stability analysis of the schemes for linear problems.

Asymptotic Preserving 2D Staggered Grid Method

Kerstin Kuepper and Martin Frank

Author keywords: transport equation, singular limit, asymptotic preserving

Abstract

We analyze a numerical method for the transport equation, which uses staggered grids for the spatial discretization. We combine a one-dimensional asymptotic preserving (AP) scheme with staggered grids by Jin (Lecture Notes for Summer School on Methods and Models of Kinetic Theory, 2010). with a special time discretization for the two-dimensional transport equation by Jin, Pareschi and Toscani (SIAM Journal on Numerical Analysis, 2000). The resulting method requires less unknowns than could naively be expected. Besides that, we formally show that the scheme has the correct diffusion limit and we provide a stability analysis. We obtain an explicit CFL condition, which couples a hyperbolic and a parabolic condition. This type of condition is common for AP schemes.

Galerkin variational integrators for solid and fluids mechanics

Mattia Penati, Edie Miglio, Nicola Parolini and Roberto Porc

Author keywords: Time integrations, geometric integrators, variational integrators, discrete mechanics, elasticity

Abstract

The general family of Galerkin variational integrators has been studied and a complete classification of such methods has been proposed. This classification is based upon the type of basis function choosen to approximate the trajectories of material points and the numerical quadrature formula used in time. This kind of numerical technique leads to the definition of arbitrarily high order method in space.

Assuming the validity of some mild hypotheses, which ensure the well posedness of continuous problem, the discrete problem has been studied, proving its well posedness and its approximation properties. Moreover the preserving properties have been extensively studied.

This kind of results are not totally new, some authors studied these methods previously. All of them developed the theory in the context of Hamiltonian mechanics. In the present work a mathematical framework will be developed in order to extend this class of geometric integrators to continuum mechanics.

Different material behaviours (like elasticity and viscosity) as well as global constraints (such as incompressibility) can be casted in this frameword. This class of methods can be used to treat conservative and dissipative

processes preserving the geometric structure of the continuous equations and the conservation laws.

The theoretical results are supported by a series of numerical simulation showing the good proporties of the advocated methods. The simulations have been performed using the FEniCS library.

In the context of SOCIS 2013 (`http://sophia.estec.esa.int/socis2013/`) some of these methods have been implemented for the Hamiltonian mechanics problems. In particular the spectral variational integrators will be part of the odepkg Octave package (`http://octave.sourceforge.net/odepkg/`). Some details of the implementation are reported in the project blog (`http://geointegratorssocis.blogspot.it/`).

High Order Asymptotic Preserving Discontinuous Galerkin Schemes for the BGK Equation

Juhi Jang, Fengyan Li, Jingmei Qiu and Tao Xiong

Author Keywords: BGK model, Navier-Stokes system, Implicit-explicit, Asymptotic preserving, Discontinuous Galerkin, Micro-macro decomposition.

In this work, we develop a family of high-order asymptotic preserving (AP) schemes to the BGK equation in the hyperbolic scaling that lead to the macroscopic models the Euler and Navier-Stokes equation in the asymptotic limit. Our approach is based on the so-called micro-macro formulation of the kinetic equation which involves the natural decomposition of the equation to the equilibrium part and non-equilibrium part. The new ingredients for the proposed methods to achieve high order accuracy are the following: we introduce discontinuous Galerkin (DG) discretization of arbitrary order of accuracy in space based on one set of computational grid; we employ high order stiffly accurate implicit-explicit (IMEX) Runge-Kutta (RK) scheme for time discretization. Numerical results demonstrating the effectiveness and high order accuracy of the proposed high order schemes are presented.

Recent advances on equilibrium problems with applications to networks

When and for whom would e-waste be a treasure trove? Insights from a network equilibrium

Tina Wakolbinger, Fuminori Toyasaki, Thomas Nowak and Anna Nagurney

Abstract

E-waste is gaining increasing importance as a secondary source for raw materials. One of the major concerns of many electrical and electronic equipment waste (WEEE) take-back schemes is whether adequate amounts of WEEE flow into the designed recycling systems. In this paper, we analyze how technical, market, and legislative factors influence the total amount of e-waste that is collected, recycled, exported and (legally and illegally) disposed of. We formulate the e-waste network flow model as a variational inequality problem. The results of the numerical examples highlight the importance of considering the interaction between the supply and the demand side for precious materials in policy-decisions. Furthermore, the results emphasize the need for cooperation between recyclers and smelters and they show possible negative consequences of the recent trend of dematerialization.

Nash equilibrium problems with uncertain data

Fabio Raciti

Author Keywords: stochastic Nash equilibrium, stochastic Variational inequality, monotone operator.

We propose a formulation of Nash equilibrium problems with uncertain data. We transform the original problem into a stochastic variational inequality in a Lebesgue space and propose an approximation procedure for the solution. Specific applications to economic and traffic problems are analysed.

Supply Chain Network Competition in Time-Sensitive Markets

Anna Nagurney, Min Yu, Jonas Floden and Ladimer Nagurney

Author Keywords: supply chains, logistics, time-based competition, game theory, variational inequalities, freight services, information asymmetry.

Timely delivery of products is essential to consumer satisfaction as well as to a company's reputation. Recent well-publicized failures in timely deliveries have demonstrated the negative practical impacts. Markets in which consumers are willing to pay a higher price for lower delivery times are referred to as being time-sensitive. In this paper, we develop a game theory model for supply chain network competition in time-sensitive markets in which consumers respond to the average time of delivery associated with the various firms' products which represent brands. The firms' behavior is captured, along with the supply chain network topologies, with the governing equilibrium concept being that of Nash equilibrium. We derive the variational inequality formulation of the equilibrium conditions and provide several illustrative examples. We also identify special cases that demonstrate how this framework may be used in distinct applications. An algorithm is proposed, with nice features for computation, and the framework further illustrated through a case study in which we explore varying sensitivities to the average time of delivery of products at the demand markets with interesting results.

Smoothed Particle Hydrodynamics and its applications

Numerical simulation of heat transfer in underground electrical cables

Sudarshan Tiwari[124], Axel Klar[125] and Steffen Hardt [126]

Abstract

We present simulations of wetting phenomena by a meshfree particle method. In this method, a flow domain is filled by a number of particles. The fluid phases are separated by assigning different colors to different subsets of particles. In addition to that, different densities and viscosities are assigned to each phase, remaining constant during the simulation. We model two-phase flow by a single-fluid description with spatially varying properties by taking the weighted average of the densities and the viscosities in the region around the interface. The flow is computed by solving the incompressible Navier-Stokes equations using Chorins projection approach. We use the CSF model for computing the surface tension force. The differential operators at each particle position are computed from its surrounding point cloud with the help of the least squares method. This an extension of our earlier works, where wetting effects have not been included. We present several numerical examples. The results are compared with analytical solutions, if available, and with other published numerical results.

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SPH for the simulation of a dam-break with floating objects

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Abstract

We show the application of the Smoothed Particle Hydrodynamics (SPH) method in the fully 3-D simulation of a dam-break on natural topography, including interaction of the fluid with moving rigid objects. Boundary conditions are computed using the unified semianalytical model proposed by Ferrand et. al [1], and include the treatment of turbulence through the Reynolds-averaged $k\epsilon$ model. The implementation is based on GPUSPH [2], an implementation of 3-D SPH in CUDA. The natural topography is imported into GPUSPH after preprocessing with Crixus, a tool that computes the initial values of the boundary integrals for the wall segments and boundary particles. Objects are discretized using boundary particles, and SPH is used to compute the interaction of fluid and object particles. The total force and torque acting on the each object is then used to integrate the motion of the object through coupling with the open-source ODE library, which also takes into account interactions between objects, and between

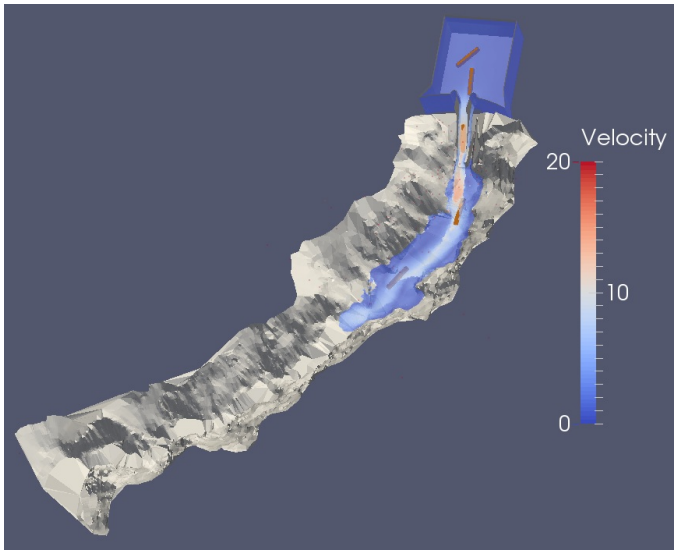

Figure 13: Dam-break on natural topography with floating trees modelled by cylinders. The water is colored by velocity magnitude.

objects and the topography.

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Full 3D numerical simulation and validation of a fish pass with GPUSPH

Eugenio Rustico (BAW, INGV), Béla Sokoray-Varga (KIT), Giuseppe Bilotta (INGV, DMI), Alexis Hérault (INGV, CNAM), Thomas Brudy-Zippelius (BAW)

As fish have a limited swimming performance, the flow velocities within the pools of a fish pass determine whether a fish can pass through the facility. Hydraulic research on vertical slot fish passes has shown that the hydraulic conditions within the pools of such facilities are affected by the pool geometry and the slope of the fish pass. CFD modeling represents an efficient tool to investigate different geometry variants. However, a validation of the model is necessary, due to the complexity and high turbulence of the flow in such facilities.

In the present paper we simulate a vertical-slot fish pass with GPUSPH, a high-performance CUDA implementation of the Smoothed Particles Hydrodynamics (SPH) numerical model for free-surface flows. While previous SPH-based approaches to the numerical simulation of fish passes were mostly in 2 dimensions, the use of SPH allows to run fully threedimensional simulations, without constraints on the domain shape and with great accuracy. This comes at the cost of significant requirements in terms of memory and computational power. To cope with this, we have extended GPUSPH, which previously supported single-node multi-GPU computing, to exploit the computational power of clusters of graphic devices. By exploiting 12 devices across 6 nodes simultaneously we have been able to run a fine-grained simulation with a resolution of about 4mm per particle and a total of 50 millions particles.

The results obtained in GPUSPH are compared to flow velocity and water level measurements from a laboratory model with identical geometry. Laboratory measurements were performed by an Acoustic Doppler Velocimeter (ADV) while the water-level measurements were obtained by ultrasonic distance sensors mounted in each pool.

The first tests show a good agreement of the simulation with the laboratory measurements. Both the distribution and the magnitude of the velocities are similar, as well as the water levels measured in the corners of the pools. Moreover, the simulation correctly reproduces the shape of the main stream and the recirculation regions in the pools as observed in the laboratory model.

Current results are very promising and further tests are being performed to better assess how numerical simulation can be of assistance in the prototyping phase of real-world application of hydraulic engineering projects.

Mathematical Methods in Photoacoustic Tomography and Optical Coherence Tomography

A Gradient Descent Method for Photoacoustic Imaging in Sound-Heterogeneous Media

T. Glatz, Z. Belhachmi and O. Scherzer [127]

Abstract

Photoacoustic imaging (PAI) is an emerging high contrast imaging technology. It utilizes the photoacoustic effect that occurs when exposing matter to a pulse of electromagnetic radiation. Depending on the amount of absorbed energy, this excitation generates an ultrasonic signal that is recorded over time by a detector array outside the object.

A widely accepted model for the propagation of the acoustic pressure can be written in terms of a wave equation initial value problem. This model describes the so-called acoustic (*qualitative*) part of the photoacoustic problem, its task is to recover the initial pressure function from the measurements taken over time on some measurement surface. In the case of constant wave speed inside and outside the specimen, analytic reconstruction formulas of Fourier and back-projection type are known in both two and three dimensions for several measurement geometries, including planar and spherical detector shapes. In case of a spatially varying speed of sound, commonly so-called time reversal techniques are used, where an initial-boundary value

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problem is solved backwards in time.

In contrast to time reversal, in our approach the PAI inversion with variable speed of sound is seen from a variational point of view, which enables us to apply convergence results from regularization theory. By employing the fact that the speed of sound is homogeneous outside some compact area of interest, we can solve the transmission problem globally by a coupled FEM-BEM method.

An optimal control problem in photoacoustic tomography

Maïtine Bergounioux

Author keywords: Photoacoustic tomography Inverse problem Optimal control

Abstract

We deal with a photoacoustic tomography model. Photoacosutic tomography is an imaging technique based on the reconstruction of an internal photoacoustic source distribution from measurements acquired by scanning ultrasound detectors over a surface that encloses the body containing the source under study. In a nutshell, the inverse problem consists in determining absorption and diffusion coefficients in a system coupling a hyperbolic equation (acoustic pressure wave) with a parabolic equation (diffusion of the fluence rate), from boundary measurements of the photoacoustic pressure.

Since such kinds of inverse problems are known to be generically ill-posed, we propose here an optimal control approach, introducing a penalized functional with a regularizing term in order to deal with such difficulties. The coefficients we want to recover stand for the control variable. We provide a mathematical analysis of this problem, showing that this approach makes sense. We finally write necessary first order optimality conditions and give preliminary numerical results.

QUANTITATIVE PHOTOACOUSTICS

Simon Arridge, Ben Cox and Tanja Tarvanien

Author Keywords: Photoacoustics, radiative transfer, non-linear optimisation, adjoint methods.

Abstract

Quantitative photoacoustic tomography involves the reconstruction of a photoacoustic image from surface measurements of photoacoustic wave pulses followed by the recovery of the optical properties of the imaged region. The latter is, in general, a nonlinear, ill-posed inverse problem, for which model-based inversion techniques have been proposed. Here, the full radiative transfer equation is used to model the light propagation, and the acoustic propagation and image reconstruction solved using a pseudo-spectral time-domain method. Direct inversion schemes are impractical when dealing with real, three-dimensional images. In this talk an adjoint field method is used to efficiently calculate the gradient in a gradient-based optimisation technique for simultaneous recovery of absorption and scattering coefficients.

An Iterative Reconstruction Formula for Optical Coherence Tomography

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Abstract

In this work, we consider the inverse scattering problem to reconstruct the susceptibility of an anisotropic dielectric dispersive medium from measurements obtained using Full-field Optical Coherence Tomography (FF-OCT). The medium is illuminated by a laser pulse and the backscattered field is combined with a reference field, back-re ected by a moving mirror (time-domain). Then, the measurements are given on the detector's surface for varying mirror's position. Assuming that the unknown susceptibility is constant over planes related to the detection points, we show that three different polarizations of the incident field uniquely determine the orthogonal projection of the two dimensional Radon transform of the susceptibility. Finally, for three rotations of the sample, an inversion of the limited Radon transform allows to recover the susceptibility.

Keywords: Inverse Problems, Optical Coherence Tomography, Reconstruction Formula, Radon transform

Advanced Imaging for Industrial Application

Iris Segmentation: a new strategy for real biometric applications

Marco Leo and Cosimo Distante[128]

Abstract

Human identification leads to mutual trust that is essential for the proper function- ing of society. With an increasing attention to security, biometric authentication has grown in popularity as an alternative way to provide personal identification that can overcome the limits of traditional authentication systems based on credentials (documents and PIN) which may be lost, stolen, or easily forged [5]. One of the most attractive and promising biometric modalities is based on the recognition of the iris texture that is stable and distinctive, even among identical twins (similar to fingerprints), and extremely difficult to surgically spoof. The fundamental components of an iris recognition system are: image acquisition, iris segmentation, iris feature extraction, iris template generation, iris template matching, and iris identification. Iris segmentation includes pupillary boundary and limbic boundary detection, and eyelids and eyelash exclusion [4] and its performances strongly affect the accuracy of the persons identification accuracy.

The most relevant and widely used algorithms require NIF camera to segment the iris images [2]. The well-known integro differential operator [3] is then used to search a circle to separate iris clearly from other parts of the imagery and remains in use widely today in commercial applications. Another classical circle-based model is the edge detection-based techniques

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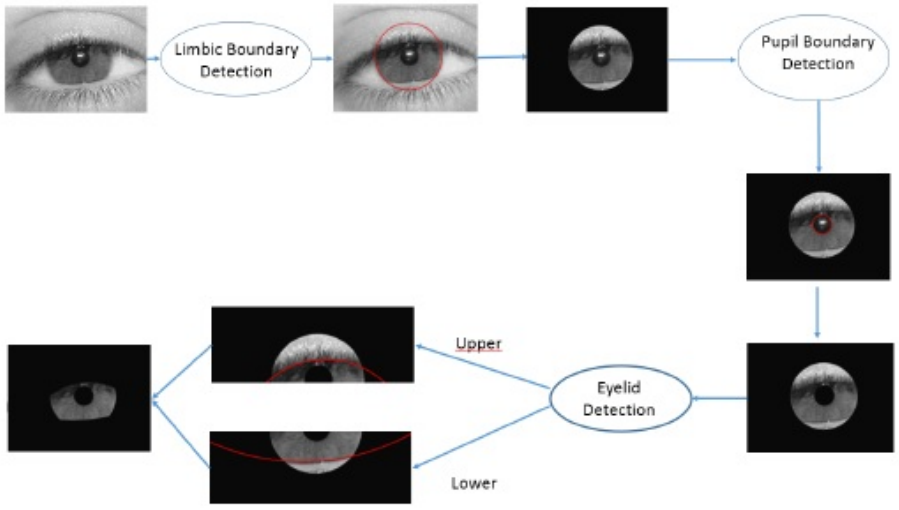

Figure 14: a schematic representation of how the proposed system works

[11], where the circular Hough transform is followed by edge detection to localise iris boundary. Unfortunately the above algorithms significantly decrease their accuracy if noisy iris images taken in visible wavelength and under non-ideal imaging conditions are used as input. In these cases, some of the factors that make the segmentation very challenging are: occlusions caused by the anatomical features of the eye (eyelids, eyelashes,...), illumination (poor illumination, specular reflections), user cooperation (off-angled iris, motion blur, eye glasses or contact lenses,...) [7]. To address such a challenge, some efforts have been recently made [1] [9] [10] and [8].

Unfortunately, most of the above segmentation schemes are very complex (many different sequential algorithmic steps involved), are not parameter free and, above all, they make use of some a priori knowledge. In other words, the experimented accuracy results on challenging datasets, are obtained through the use of specific optimizations which reduce the usability in real identity check applications.

Starting from these considerations, this paper aims at introducing an iris segmentation algorithm that overcomes some of the aforementioned limitations of the state of the art methods. The proposed approach works on input iris image taken in visible wavelength. In figure 14 a schematic representation of how the system works is reported.

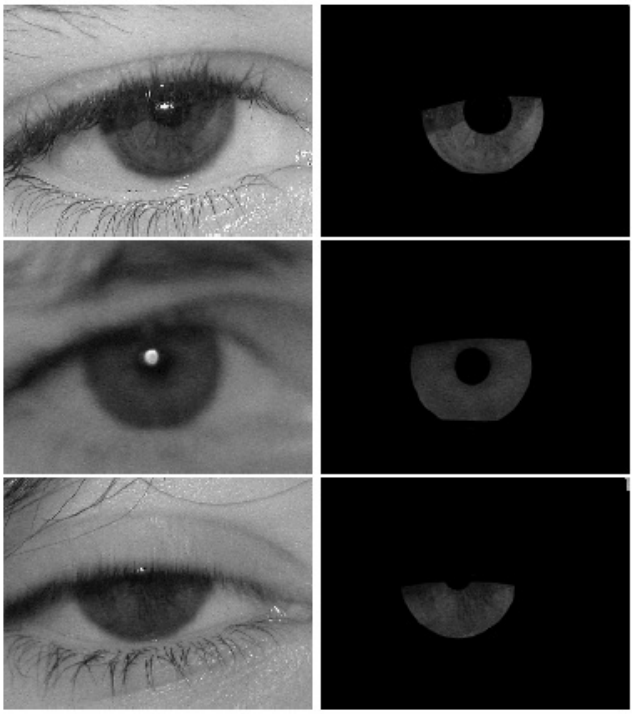

Figure 15: Segmentation results on the UBIRISv1 dataset (Session 1)

Its algorithmic core is a randomized circle detection algorithm which uses an alternative multiple-evidence strategy to define a valid circles set. The algorithm is iteratively applied to find limbic, pupil and eyelid boundaries. The proposed segmentation scheme can be used in unconstrained environments, under non-ideal imaging conditions, and above all it does not require any interaction for adaptation to different operating conditions. This has been widely proved by testing it on challenging datasets containing noisy image and by comparing its outcomes with those of the leading approaches in literature.

Figure **??** shows the segmented images after applying the proposed iris segmentation algorithm on session 2 of the UBIRISv1 database [6].

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Web Scraping of online newspapers via Image Matching

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Abstract

Reading is an activity which takes place widely on the web: every newspaper in the world has his own digital version on the internet and there are even a lot of magazines that exist only on the web. In such a scenario, Computer Vision can offer a useful set of tools that can help web editors to improve the quality of the provided service. One of these tools is here presented: given a webpage of a newspaper or journal, the proposed framework localizes news items remotely clicked by users, giving the bounding box of the content of an article in its relative homepage. The tool is hence able to track an article in the page in which is contained at any time during the day: such an information is very useful for web editors to understand the trend of the published items and to rearrange the contents of the homepage accordingly.

The system has been developed with an hybrid approach: first we manipulate the HTML source of the homepage in order to generate a visual template for the news item we want to localize. A visual template for a news item is an HTML document containing only the displayed content of the article in the homepage, that is the text of the title and the image attached to the article, if any. The algorithm which builds the template needs just the URL of the article. Thereafter, we take the screenshot of the template in order to get an image representing the news. On this image, we extract

FAST keypoints [1], which fit well for the kind of images we are dealing with, that is almost blank images mainly composed of text. The keypoints extraction is done also for the screenshot of the homepage at system start time: therefore, we can now match the article image with the homepage image and get the bounding box of the news in its parent webpage. We provided four keypoint descriptors for the matching: SIFT [2], SURF [3], BRIEF [4], BRISK [5].

We also implemented articles localization via Template Matching, using the Normalized Correlation Coefficient as measure of similarity. In order to ensure the matching, we have to discard all the redundant blank content placed on the borders of the image, given by the fact the picture comes from a screenshot. We use the extracted keypoints for this purpose: since FAST keypoints are located only upon non blank parts of an image, we can use the bounding box containing them to cut the picture and remove the void borders.

We tested the system by labelling the bounding boxes for all articles for a set of websites. Then, we compared the extracted rectangles with the ones of the ground truth. We compared the performances of Template Matching versus Keypoint Matching using the aforementioned descriptors. For each extracted bounding box, we measured the euclidean distance of its center from the corresponding rectangle center of the ground truth; for each test, we provide evaluation measures to assess the accuracy of the developed algorithm. Also, we provide HIT/MISS.

The results depend on the layout of the websites and on the manner they arrange the contents in the homepage. Our tests show that good performances can be reached, giving also an interesting case of comparison among different keypoint descriptors.

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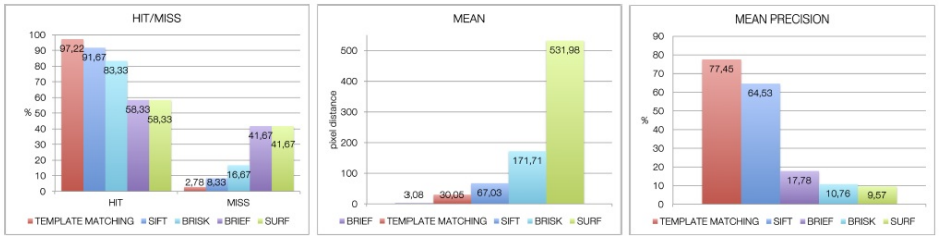
Figure 16: Localization and bounding box generation example from the homepage of Repubblica (`www.repubblica.it`). On the left side is shown a portion of the screenshot of the homepage; on the right side is shown a portion of the screenshot of the generated template for the localized article. The coloured lines show the matching between FAST keypoints in the two images. In this case, SIFT descriptor has been used for the matching.



(a) Hit and miss (b) Mean localization error (c) Mean precision

Figure 17: Test results from the National Geographics italian homepage (`www.nationalgeographic.it`). Hit and Miss (a) are calculated by measuring the ratio between unions and intersections among the ground truth rectangles and the ones coming from the test. Mean precision chart (c) shows the mean of such ratio, that is the average amount of overlapping area between ground truth bounding boxes and the corresponding ones generated by our system.

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A customized system for vehicle tracking and classification

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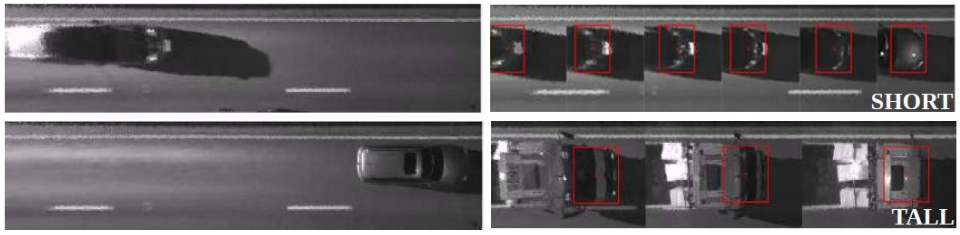
Abstract

We present a customized system for vehicle tracking and classification. The main purpose of the system is tracking the vehicles in order to understand lane changes, gates transits and other behaviors useful for traffic analysis. The classification of the vehicles into two classes (short vehicles vs. tall vehicles) is also performed for electronic truck-tolling as well as to optimize the performances of the tracker module. The whole system has been developed through a data driven approach based on video sequences acquired by QFree[129]. The sequences are acquired by wide angle cameras from the top of the road and are preprocessed in order to obtain a normalized, lowresolution representation of the scene where the distance between neighboring pixels is constant in the real world. The sequences exhibit high variability in terms of lighting changes, contrast changes and distortion. We assume that the vehicle detection is performed by an external module for plate recognition.

[129] Q-Free (`www.q-free.com`) is a global supplier of solutions and products for Road User Charging and Advanced Transporation Management having applications mainly within electronic toll collection for road financing, congestion charging, truck-tolling, law enforcement and parking/access control.



The tracking algorithm is based on Template Matching [1,2] and the Normalized Cross Correlation is used as similarity measure. The vehicle template is updated at each frame to cope with the vehicles' changes of appearance. In order to deal with the main variabilities, four modules are designed: a multicorrelation module to deal with the appearance of artifacts on the vehicles; a refinement module to deal with the change of the vehicle horizontal scale due to distortion; a background subtraction module to deal with perspective issues on tall vehicles; a selective update module to avoid the propagation of a wrong template in the slow scenes. A controller has been realized to switch on or off the modules depending on the vehicle estimated speed and the vehicle estimated class. Two measuring methods are defined to assess the performances of the proposed tracker with respect to other standard tracking pipelines [3-6] in a supervised way. The performance analysis points out that the vehicles are correctly tracked for nearly the 99% of the scene.

The classification is performed when the vehicle approaches the central part of the scene, where the variabilities are less significant. The image patches are extracted from the frame taking into account the estimated vehicle bounding box. The training set is built considering the image patches extracted from the input sequences. To make the learning procedure more robust, the training set is augmented generating artificial patches tailored to introduce alignment, perspective, rotation and photometric variabilites. The patches are normalized to the training set mean patch size and the HOG (Histogram of Oriented Gradients) features are extracted [7]. The feature vectors dimensionality is reduced through the Principal Component Analysis (PCA) [8]. The labeled samples are then projected through the Linear Discriminant Analysis (LDA) [9] to the most discriminant dimension. This unidimensional feature is aggregated to the patch height in pixels, obtaining a two-dimensional vector. A new LDA projection is hence performed on the twodimensional samples and the two projected populations are modeled as unidimensional Gaussian distributions. In the classification step, the sample

is projected using the previously learned PCA and LDA bases. The Mahalanobis distances [10] are computed between the projected sample and the Gaussian distributions related to the two classes (short vs. tall vehicles). The sample is assigned to the class giving the smallest distance. The classification performances are evaluated with the Leave One Out strategy and the overall classification accuracy is over the 98%.

This work has been performed in the project PANORAMA, co-funded by grants from Belgium, Italy, France, the Netherlands, and the United Kingdom, and the ENIAC Joint Undertaking.

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Optimization and Optimization-based Control Methods for Industrial Applications

Distributed Model Predictive Control for a Smart Grid Application

Karl Worthmann, Christopher Kellett, Philipp Braun, Lars Grüne and Steven Weller

Author keywords: model predictive control, smart grid application, distributed control

Abstract

Residences with small-scale solar electricity generation such as roof mounted solar photovoltaic panels are becoming increasingly common. Alongside the positive effects of switching from fossil fuels to renewable resources, the change from centralized electricity generation to small-scale distributed electricity generation imposes many challenges to electricity distribution networks designed for one-way power flow from the distribution company to the residential customer. In particular, during periods of high generation and low load, reverse power flows can lead to degradation of power quality and overvoltage conditions leading, in the worst case, to power outages. To address these challenges, installation of distributed battery storage into the network is increasingly being considered to reduce variability in power supply and demand.

In this work, we consider a small neighborhood-level electricity network consisting of a single grid provider and several residences with batteries and solar panels. We present model predictive control approaches, namely centralized, distributed and decentralized, to find optimal charging/discharging

strategies for distributed battery storage that help to mitigate the negative effects of small-scale renewable generation.

The distributed model predictive control algorithm is based on a so-called market maker, a concept from financial mathematics, with the idea to achieve the mentioned goals by iteratively setting the prices for buying and selling electricity within the network. Our results are illustrated using real world data on generation and load profiles provided by an Australian electricity distribution company.

A optimization method for piecewise linear problems

Sabrina Fiege, Andreas Griewank and Andrea Walther

Author keywords: Lipschitzian optimization problems, bundle methods, piecewise linearization

Abstract

Nonsmoothness is a typical characteristic of numerous objective function in optimization that arises from various applications. We present an optimization method based on algorithmic or automatic differentiation (AD) for piecewise linear (PL) functions. Because the nondifferentiabilities are caused by the occurrence of the absolut value function in many realistic cases, we concentrate on these functions.

This work is motivated by examples of convex unconstrained minimization problems, where the steepest descent method with exact line-searches exhibits zigzagging convergence to a non-stationary point. Such a behavior is known as Zeno behavior in the switching system theory. In particular, we consider an convex example that can be found in Convex Analysis and Optimization Algorithms by J.-B. Hiriart-Urruty and C. Lemarechal. There one can also find that the continuous steepest descent trajectory defined by the differentiable inclusion converges to a stationary point and thus is a minimizer if the function is convex and bounded below.

Stationarity and first order minimality of PL functions f at a given point x is analyzed and an algorithm to decide whether these properties are attained will be presented. The stationarity test uses a bundle G which is a subset of the Clarke generalized gradient of f at x and yields a descent

direction if the test fails. Furthermore, a test for convexity at a point x can be performed.

Subsequently, to optimize a PL function it is superimposed by a proxmial term. The arising structure of the function domain will be exploited in that the required information as the direction of descent, the generalized gradient etc on an open polyhedron will be studied. In the convex case the method converges to a minimum whenever the PL functions are bounded below and it can also be shown, that the method converges after finitely many steps. For the non-convex case the latest results of the analysis of convergence will be presented.

This talk presents numerical results for the convex and non-convex case. Additionally, a first application from economies will be introduced.

Our future goal is to optimize piecewise smooth functions which we repeatedly approximate by a local piecewise linearization. By doing so, we reduce the piecewise smooth case at the current iterate to the PL case by adding an additional outer loop.

Computational Aspects of Optimization-Based Path Following of an Unmanned Helicopter

Johann C. Dauer[130] and Timm Faulwasser[131] and Sven Lorenz[132]

Abstract

In this paper we consider the path following of unmanned helicopters based on dynamic optimization. We assume that the helicopter is equipped with a flight control system which provides an approximation of its closed-loop dynamics. The task at hand is to derive inputs for this flight control system in order to track a geometrically specified path.

We present a concise problem formulation and discuss an efficient implementation. This implementation achieves computation times below the flight duration of the path by exploiting differential flatness of components of

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the dynamics. Finally, we present quantitative results in respect to convergence and required iterations for a challenging nonlinear path.We show that the proposed optimization based approach is capable of tackling nonlinear path following for helicopters in an efficient manner.

Logistics Driven Requirements and Limitations to Model Predictive Control

Jürgen Pannek

Author Keywords: model predictive control, supply chain management, distributed control, Lyapunov stability, feasibility.

Abstract

Supply chains management deals with the problem of transportation of goods across a network from suppliers via production, distribution and storage facilities to retailers and costumers. While several different companies may be interacting in such a setting, house supply chain management focuses on the network within only one company. The advantage of this cutout is the availability of information for all nodes in the chain, and the accessibility of both the control and information structure. Here, instead of known strategies such as postponement, we propose a model predictive control (MPC) scheme to obtain such a controller. Since the network may be large, we pursue a distributed approach, i.e. each node in the network is locally controlled. A respective implementation optimizes a cost criterion subject to the local dynamic and local and shared constraints. To coordinate the feedbacks, only the changeable information structure is used. In the algorithmic global view, we analyze the interplay between the two key components optimization and coordination with respect to stability properties in the sense of Lyapunov for the overall closed loop. In particular, we follow the approach

of [1] and propose a distributed model predictive control algorithm, which is based on exchange of primal variables and tailored for the requirements of in house supply chain management. Although we avoid the use of stabilizing terminal constraints or costs, cf. [2] for the supply chain case, we provide feasibility and stability results for the proposed setting. To this end, we utilize a trajectory based stability result, which additionally allows us to bound the tradeoff between the distributed MPC implementation and the infinite horizon optimal control. Last, we discuss the information related in house supply chain limitation of the approach and point out possible solutions.

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Mathematical Applications to an Unmanned Aerial Vehicle

Valeria Artale, Cristina L. R. Milazzo, Calogero Orlando, and Angela Ricciardello[133]

Abstract

In this work, results obtained by the flight control simulations of a prototype of hexarotor Unmanned Aerial Vehicle (UAV) are shown. The mathematical model and control of the hexacopter airframe is presented. In particular, the sixrotors are located on the vertices of a hexagon and they are equidistant from the centre of gravity; moreover, the propulsion system consists of three pairs of counterrotating fixed-pitch propellers in order to balance the torque actions. In order to stabilize the entire system, Linear Quadratic Regulator (LQR) control is used in such a way to set both Partial Derivative (PD) and Partial Integral Derivative (PID) controls in position variables. A simulation set is performed to carry out the results for linear and non linear models. The simulations are performed to show how LQR tuned PD and PID controllers lead to zero the error of the position along Z earth direction, stop the rotation of UAV around body axes and stabilize the hexarotor. Moreover, the obtained LQR-PD and LQR-PID controllers have been tested by comparing the response to an impulse disturbances of the nonlinear dynamical system with the response of the linearised one. This work is supported by the PO. FESR 2007/2013 subprogram 4.1.1.1 *Actions*

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to support the research and experimental development in connection with the production sectors, technological and production districts in areas of potentiality excellence that test high integration between universities, research centers, SMEs and large enterprises; (Prog. *Mezzo Aereo a controllo remoto per il Rilevamento del TErritorio - MARTE* Grant No.10772131). The aim of the project is to realize a new platform for the representation of the terrain in a georeferenced raster map by using free and open source Geographic Information System (GIS). The flight control system proposed in this talk will be validated by means of a wide experimentation by using the realized prototype.

Periodic Stochastic Model Predictive Control applied to Building Temperature Control

Milan Korda and Faran A. Qureshi and Tomasz T. Gorecki and Colin N. Jones[134]

Abstract

With the decline in fossil fuel reserves and an increase in the total energy consumption, the need for energy conservation has emerged as a major challenge faced by our society. Buildings account for about 40% of the total energy consumption worldwide [3], therefore energy efficient control of building heating, ventilation, and air conditioning (HVAC) system is imperative. Model Predictive Control (MPC) has been demonstrated to improve the energy efficiency of the building HVAC operation [4]. MPC is particularly suitable for building control because of its natural ability to handle comfort constraint, and to incorporate the future weather and occupancy prediction in the controller. The weather and occupancy are stochastic in nature, and have a significant effect on the performance of the MPC controller. Moreover, these environmental factors affecting the building are also strongly periodic. This calls for control schemes which explicitly take into account the periodicity and the stochasticity of the disturbances.

In this contribution we combine the ideas of [2] and [1] to develop a periodic stochastic model predictive control (PSMPC) scheme. Similarly to

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[2], the scheme takes explicitly into account the past behavior of the constraint violation process in order to dynamically tighten/loosen the state constraints, hence allowing the control system to better exploit the freedom provided by a stochastic constraint specification. Similarly to [1], we deal with linear systems with periodic dynamics, constraints and stochastic disturbance. The proposed scheme comes with recursive feasibility guarantees of the underlying optimization problem, and guarantees on the average amount of constraint violation of the state process in closed-loop. The violation amount is measured by a user-specified loss function, which makes the approach highly flexible, allowing for a wide range of constraint specification to be handled.

The proposed PSMPC scheme is applied to achieve an energy efficient control of a building HVAC system in the presence of stochastic weather and occupancy prediction. The results are compared with existing building controllers.

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Multiobjective optimal control methods for the development of an intelligent cruise control

Michael Dellnitz, Julian Eckstein, Kathrin Flaßkamp, Patrick Friedel, Christian Horenkamp, Ulrich Köhler, Sina Ober-Blöbaum, Sebastian Peitz, Sebastian Tiemeyer[135]

Abstract

During the last years, alternative drive technologies, for example electrically powered vehicles (EV), have gained more and more attention, mainly caused by an increasing awareness of the impact of CO_2 emissions on climate change and by the limitation of fossil fuels. However, these technologies currently come with new challenges due to limited lithium ion battery storage density and high battery costs which lead to a considerably reduced range in comparison to conventional internal combustion engine powered vehicles. For this reason, it is desirable to increase the vehicle range without enlarging the battery.When the route and the road slope are known in advance, it is possible to vary the vehicles velocity within certain limits in order to reduce the overall drivetrain energy consumption. This may either result in

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an increased range or, alternatively, in larger energy reserves for comfort functions such as air conditioning.

In this presentation, we formulate the challenge of range extension as a multiobjective optimal control problem. We then apply different numerical methods to calculate the so-called Pareto set of optimal compromises for the drivetrain power profile with respect to the two concurrent objectives battery state of charge and mean velocity. In order to numerically solve the optimal control problem by means of a direct method, a time discretization of the drivetrain power profile is necessary. In combination with a vehicle dynamics simulation model, the optimal control problem is transformed into a high dimensional nonlinear optimization problem. For the approximation of the Pareto set, two different optimization algorithms implemented in the software package GAIO are used. The first one yields a global optimal solution by applying a set-oriented subdivision technique to parameter space. By construction, this technique is limited to coarse discretizations of the drivetrain power profile. In contrast, the second technique, which is based on an image space continuation method, is more suitable when the number of parameters is large while the number of objectives is less than five. We compare the solutions of the two algorithms and study the influence of different discretizations on the quality of the solutions.

A MATLAB/Simulink model is used to describe the dynamics of an EV. It is based on a drivetrain efficiency map and considers vehicle properties such as rolling friction and air drag, as well as environmental conditions like slope and ambient temperature. The vehicle model takes into account the traction battery too, enabling an exact prediction of the batterys response to power requests of drivetrain and auxiliary loads, including state of charge.

Global Multiple Shooting for Hybrid Dynamical Systems

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A standard technique for solving boundary value and optimal control problems of ordinary differential equations is multiple shooting, which reduces the problem that involves ODE dynamics to a problem of numerical optimization. In our talk we will present a multiple shooting based algorithm that solves the following extended boundary value problem:

Given:

- a hybrid dynamical system H (i.e., a dynamical system whose continuous behavior is governed by ordinary differential equations, but that, in addition, also has discrete state that may evolve in a discrete way)
- a set of initial states I
- a set of states U considered to be unsafe

Find: a trajectory of the hybrid dynamical system H that starts in the set I and reaches the set U (in the following we will call such a trajectory an *error trajectory*).

Here, in contrast to classical boundary value problems,

- we consider hybrid dynamical systems instead of ordinary differential equations,
- we do *not* fix the length of the trajectory we search for, but search for an error trajectory of arbitrary length, and

- we are not satisfied with local search, that is, with an algorithm that finds an error trajectory if started with an initial guess close enough to an error trajectory, but we search for an error trajectory globally.

Those three extension are important, since in industrial applications

- we might have systems with partially discrete behavior, for example, due to switches that might be turned on and off,
- we might not a priori know an upper bound on the length of potential error trajectories, and
- we might not have a good initial guess for an error trajectory.

In the talk we will present a multiple-shooting based algorithm that solves this problem, we discuss its properties, including a proof of convergence, and show the results of numerical experiments with a concrete implementation.

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Modeling and Optimization of Interacting Particle Systems

Optimal Control Of Interacting Particle Systems With External Agents

Claudia Totzeck

Abstract

We are considering interacting particle systems, especially under the in uence of external agents. One may think of a herd of sheep that is regulated by a dog. Optimal control problems of these systems are considered in combination with model hierarchies. How do limits that occur when passing from one model to another in uence the solutions of optimal control problems? The interesting questions arising from these settings are investigated analytically with help of asymptotic analysis and numerically.

A different perspective on Riemann problems

Jochen Kall

Author keywords: Hyperbolic conservation laws, Riemann problem, Shallow water equations, Networks, Coupling

Abstract

We present a different, Godunov state centric, perspective on the Riemann problem examplatory for the shallow water equations. We treat the Riemann problem as a particular case of a more general coupling problem with algebraic coupling conditions. Furthermore, we show how this can be applied to construct numerical schemes for hyperbolic conservation laws on networks.

Interacting particle systems for swarming and their kinetic PDEs

Stephan Martin

Author keywords: Interacting particle systems, swarming, mean-field limits, collective behavior, coherent pattern formatio

Abstract

The complex collective behavior of animals in swarms such as fish schools and bird flocks exhibits the emergence of macroscopic patterns from seemingly local interactions. Interacting particle system and their continuum limiting PDEs provide a mathematical modeling framework for such social interactions, also frequently used in crowd dynamics, opinion formation and cell biology. I will present some recent results on the analysis of particular solutions and show how seemingly small parameter changes in the models can have a strong effect on the properties of coherent patterns. Our goal of the session is also to discuss some aspects of the largely open problem of optimization and control of swarms and other applications.

From discrete to continuum in stochastic models of diffusion of finite-size particles

Maria Bruna and Jon Chapman

Author Keywords: Brownian motion, Fokker-Planck equation, Stochastic simulations, Excluded-volume effects

In this talk we will discuss nonlinear Fokker-Planck models describing diffusion processes with particle interactions. These models are motivated by the study of systems in biology and ecology composed of many interacting individuals, and arise as the population-level description of a stochastic particle-based model. In particular, we consider a system finite-sized hard-core interacting Brownian particles and use the method of matched asymptotic expansions to obtain a systematic model reduction. The result is a nonlinear Fokker-Planck equation, with the nonlinear term accounting for the size-exclusion interactions. The ability of this equation to describe the system is tested by comparing its solution against stochastic simulations of the particle-level model. As an extension, we consider a system with two interacting species (of different sizes and diffusivities) and study how the inter-species competition emerges at the population level.

Mean field game approaches in pedestrian dynamics

Martin Burger, Marco Di Francesco, Peter A. Markowich and Marie-Therese Wolfram

Author Keywords: Mean field games, Crowd motion, Optimal control, Numerical simulations

The dynamic motion of large human crowds is an ubiquitous phenomena in everyday life. First empirical studies on crowd motion started in the late 1950ties and spread into different fields like transportation research, psychology or urban and regional planning. Recently there has been a strong interest in crowd motion within the mathematical community, which initiated a lot of research on mathematical models, their analysis and simulations. In this talk we focus on a fast exit scenario and consider a group, which wants to leave a room as quickly as possible. We present different modeling approaches, starting on the microscopic level and working our way up to the appropriate continuum limits. In particular we focus on Hughes model for pedestrian flow and give an interpretation from the mean field game perspective. Finally we discuss different challenges in the analysis and numerical simulations and illustrate the behavior of the presented models with numerical simulations.

Optimal control for semiconductor diodes design based on the MEP energy-transport model

Drago Concetta and Romano Vittorio

Author Keywords: Optimal semiconductor design, adjoint method, MEP energy transport.

An optimal control approach based on the adjoint method is performed for the design of a semiconductor device by using a consistent energy transport model, free of any fitting parameters, formulated on the basis of the maximum entropy principle (MEP). Optimal design of silicon n+-n-n+ diodes and comparisons with the results obtained by using standard energy-transport model, known in literature, are shown.

Multiphysics simulations with industrial applications

The optimisation of tidal turbine arrays

Patrick Farrell and Simon Funke

Author Keywords: optimization, adjoint, FEniCS, shallow water, turbines, industrial design

Abstract

Just as wind turbines extract energy from the kinetic motion of the atmosphere, tidal turbines extract energy from the movement of the tides. This resource has great promise, but several major problems must be solved before large arrays can be deployed. One such problem is deciding how to configure them: how should the turbines in an array be placed to extract the maximum possible energy? The configuration makes a major difference to the power extracted, and thus to the economic viability of the installation.

In this talk, I present the modelling and formulation of this question as a PDE-constrained optimisation problem, and present some initial solutions for the design of an array of tidal turbines to be deployed off the north coast of Scotland in 2018.

Finite-element/boundary-element coupling for inflatables

Timo Van Opstal and Harald Van Brummelen

Author Keywords: Finite element method, Boundary element method, Fluid-structure interaction, Large displacements, Strong coupling.

In a small percentage of airbag deployments, out-of-position impact occurs, usually resulting in severe injuries. To understand and improve the inflation process, a precise understanding of the airbag dynamics is required. This can be provided by accurate numerical simulations. These simulations are however a complicated endeavor, mainly on account of the large displacements and length-scale disparities inherently involved. On the one hand, a realistic stowed airbag constitutes a labyrinth of intricate folds. On the other, the final configuration is a relatively simple bulb. To date, the complex behavior on the small scales has been overly simplified, rendering the results inappropriate for analysis of out-of-position situations. The approach proposed here is to identify subdomains of the fluidic domain amenable to resolution of the small scales. The boundary element method is very suitable for the discretization of these geometrically complex folded subregions for a number of reasons:

- no initial volume mesh need be generated, as the structure mesh can be inherited by the fluid;
- the large displacements do not entail mesh skewing as the mesh automatically tracks the structural motion;
- the solution is calculated exclusively where it is required: at the coupling interface.

On the down side, dedicated numerical schemes are required to evaluate the involved singular integrals, and the resulting matrix system is full if no special measures are taken. This method, which was explored in the planar setting (c.f. [3]), is now extended to the three-dimensional setting. The interior Stokes flow [2] is discretized by the boundary element method. The inherent lubrication effect is exploited to inhibit self-intersection of the structure. This feature of Stokes flow is also utilized to prevent exterior contact by solving the exterior problem simultaneously, at no extra cost. The structural motion is governed by the Kirchhoff-Love shell model [1]. Numerical examples are given to demonstrate the performance of the proposed scheme.

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Optimal Shunt Placement for Hydrocephalus Treatment via Patient-Specific, Multiphysics Simulations

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Keywords: multiphysics simulations; patient-specific treatment; optimal shunt placement; hydrocephalus; mesh warping; level sets

Abstract

Hydrocephalus is a neurological condition caused by abnormalities in the cerebrospinal fluid (CSF) flow. As a result, the brain ventricles dilate, and the tissue compresses, which causes physical and mental problems. One popular treatment of hydrocephalus has been the surgical implantation of a CSF shunt in the brain ventricles in order to divert the CSF flow. However, the outcomes of this therapy (and others) continue to be poor. Thus, there is a need for improved treatment protocols to be designed.

An important first step towards this goal is the development of predictive computational models for the mechanics of hydrocephalic brains. Unfortunately, existing mechanical models of hydrocephalic brains are rather simplistic and fail to explain the mechanisms governing the development of hydrocephalus. In the absence of sophisticated mechanical models, we have developed a geometric approach for simulation of the evolution of the

brain ventricles and CSF. In our prior work, we proposed a combined level set/mesh warping algorithm in collaboration with Jeonghyung Park in [1,2]. We have successfully used our algorithm to track the evolution of the brain ventricles and CSF before and after shunt implantation in hydrocephalic patients.

In this talk, we will describe our results obtained from patient-specific simulations of optimal shunt placement in hydrocephalic patients. Our patient-specific simulations are multiphysics in nature in that the onset and treatment of hydrocephalus involve aspects of CSF production, transport, and absorption in addition to brain tissue compression. The simulations make use of our combined level set/mesh warping algorithm in order to track the evolution of the brain ventricles and CSF in response to various shunt placements. Such simulations can be of use to neurosurgeons when determining where to surgically implant a CSF shunt in a hydrocephalus patient.

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Mathematical Characterization of a Heat Pipe by means of the Non-Isothermal Cahn-Hilliard Model

Melania Carfagna, Filomena Iorizzo, Alfio Grillo [136]

Key words: Heat pipes, Non-isothermal Cahn-Hilliard Model, Mixture Theory

Heat pipes are two-phase heat-transfer devices widely used in Industrial Engineering, since they efficiently transfer large amounts of heat. A heat pipe consists of a vacuum sealed hollow tube in which a small amount of fluid experiences phase changes from the liquid to the vapour phase and vice versa. To allow these phase changes, the pipe is heated at one of its two ends, where the fluid absorbs the necessary latent heat to evaporate, and it is cooled down at the other end to let the vapour condensate. This way of supplying and subtracting heat and the presence of a wick structure,

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which covers the internal wall of the tube, generate a motion of the two-phase (liquid/vapour) fluid hosted in the pipe. Indeed, this wick structure supports the reflux of the condensate liquid unto the heated zone by means of a capillary action.

The heat pipe performance is generally investigated by means of lumped parameter models or simplified thermal hydraulic models. The purpose of this work is to *take a look* inside this heat exchanger to verify its working conditions, focusing the analysis on an all-embracing thermo-fluid dynamic behaviour of the liquid/vapour pair inside the pipe [1]. The mathematical description of the twophase system inside the heat pipe has been obtained by manipulating the Cahn-Hilliard model for phase transitions and setting it into the framework of Mixture Theory [2]. This approach leads to a thermodynamically consistent set of five coupled, highly non-linear partial differential equations accounting for:

1. Evaporation and condensation, depending on the temperature and the pressure of the system in the different zones of the tube;

2. The presence in the field equations of non-standard terms that define the strong coupling between thermal and mass fluxes [3].

The resulting non-isothermal Cahn-Hilliard model, as applied in the current effort, was examined by means of numerical full-scale axi-symmetric simulations of the heat pipe working in micro-gravity conditions.

This study was developed in cooperation with Argotec s.r.l., an Aerospace Engineering company, which provided also experimental data to validate the model. The numerical results are in good agreement with the experimental data.

Further refinements of both the model and the related numerical procedures are subject of our current investigations.

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An Optimal Control Approach to Full Waveform Inversion (FWI)

Marianna Signorini, Stefano Micheletti and Simona Perotto

Author Keywords: Wave equation, absorbing boundary conditions, optimal control.

Abstract

We consider an optimal control approach applied to the theory of Full Waveform Inversion (FWI) in time domain using the Lagrangian method (or optimal control)for acoustic waves in isotropic elastic media. As a reference geophysical setting we consider shots and receivers placed just underneath the Earth surface. The goal of the analysis is to locate the subsurface reflectors and to determine the soil profile. In order to achieve this goal, FWI minimizes the misfit between the recorded and the numerical pressure at the geophones. It is known that this minimization problem is ill-posed. For this reason the cost functional is regularized with the addition of suitable penalization term. We use a finite difference scheme in space and a leap frog method in time in order to discretize the wave equation and the Barzilai-Borwein method to minimize the cost functional. We compare the results obtained with both reflecting and absorbing boundary conditions and with different regularization terms.

Numerical and constitutive aspects of the cardiac electromechanical coupling

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Abstract

Heart failure (HF) is one of the major challenges in modern cardiology. An effective treatment for HF patients can be cardiac resynchronization therapy (CRT). Unfortunately, current diagnostic tools are clinically insufficient to guide clinicians in the optimal application of CRT, as testified by the high percentage of non-responding patients to the therapy (up to 30%).

Over the last decade, several research groups have been working on modeling CRT by combining patient-specific geometrical, electrical and mechanical information. Such models can potentially improve the diagnosis. On the other hand, modeling the heart dynamics is a complex multiphysics problem, spanning several temporal and spatial scales. Thus it is not a trivial task to build consistent mathematical models and robust numerical schemes.

The first part of this work is devoted to the numerical discretization of electrophysiology models, which are composed by a reaction-diffusion equation coupled with a generally large set of ODEs. The dynamic behavior, characterized by a steep traveling front wave, requires a computational grid of the order of 200 μm or less, yielding considerable computational efforts on human geometries. We show how specific discretization schemes (finite difference, continuous and discontinuous finite element, etc.), and the choice of a coarse grid, can assect the solution, leading to possibly erroneous physiological conclusions. Moreover, we explore and suggest different strategies

to address the issue.

In the second part we focus on modeling the active mechanical behavior of the heart. The shortening of the myocardial fibers is the microstructural engine that produces the contraction of the cardiac muscle. The complex interplay between fibers shortening and elastic macroscopic strain is functional to the ejection of blood into the arterial network. Here we address the contraction of the left ventricle in a finite elasticity framework, adopting the invariants-based strain energy proposed by Holzapfel and Ogden, where the mechanical role of fibers and sheets are accounted for. We show that a model based on multiplicative decomposition of the deformation gradient is able to reproduce P-V loop, muscle torsion, transmural strains and the overall motion, without introduction of any further *ad hoc* law.

We conclude with quantitative results generated from a strongly coupled model of cardiac electromechanics, in which the equations of electrophysiology and mechanics are solved fully coupled. The results are summarized and discussed in the context of physiological and clinical relevance.

A reduced nonlinear model for the simulation of two phase flow in a horizontal pipe

Matteo Pischiutta and Gianni Arioli

Author Keywords: two phase flow, multiphase flow, horizontal pipe, reduced model.

Abstract

There exist many 3D numerical schemes to study the flow of a mixture of liquid and gas in a pipeline, but although they offer a very good accuracy, they are rarely fit for modeling a long pipe, due to the high computational costs. Then one is usually led to consider 1D models, see e.g. the works of Issa and his group. Such models offer much faster simulations than 3D schemes, on the other hand they almost completely miss the dynamics in the transversal direction. Here we present a model able of representing the full 3D dynamics, but with the computational cost typical of 1D simulation. The main feature of our model consists in describing the dynamical variables in the direction transversal to the pipe by means of a family of functions depending on a set of parameters. The model is then solved by a standard finite volume scheme.

Field application of groundwater flow data assimilation through Moment Equation based Ensemble Kalman Filter

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Symposium n^o 53: *Multiphysics simulations with industrial applications.*

Keywords: Data assimilation, EnKF, Transient groundwater flow, Moment equations, Aquifer characterization

Conditioning the spatial distribution of the petrophysical properties of aquifer systems (i.e., permeabilities and porosities) on the basis of available direct or indirect/surrogate measurements is a key step to improve our ability of providing appropriate predictive models of flow and transport phenomena occurring in the subsurface environment. The Ensemble Kalman Filter (EnKF) is a valid tool in this context. It allows assimilating data into (generally non-linear) models sequentially, as soon as they become available. The EnKF has traditionally entailed the use of Monte Carlo (MC) simulations to generate a collection of calibrated model realizations. In many practical applications, the computational burden associated with

this approach requires limiting the size of the MC sample, rendering spurious covariances and incorrect parameter updates. Recently, we developed a novel data assimilation technique which is grounded on coupling the EnKF algorithm with a set of moment equations (MEs) governing the space-time dynamics of (ensemble) mean and covariance of groundwater flow state variables (hydraulic heads and fluxes). This methodology allows circumventing the need for MC simulation in the EnKF algorithm. The accuracy and the feasibility of the ME-based assimilation scheme has been successfully tested through a suite of synthetic studies and has been demonstrated to be a viable alternative to MC both in terms of computational efficiency and accuracy of the calibrated models. In this work we consider the application of our new ME-based EnKF to a set of cross-hole pumping tests performed at the Lauswiesen test site, near Tbingen (Germany). We assimilate the available measurements through our methodology with the objective of characterizing the spatial distribution of the log-transmissivities (Y) over the domain of interest. We test the quality of the calibrated model by comparing the drawdowns calculated on the basis of the estimated mean and covariance spatial distributions of Y against measured values acquired during an independent pumping test which was not considered in the assimilation procedure.

Numerical Treatment of High Index Dynamical Systems

Andreas Steinbrecher

Author Keywords: dynamical systems of high index, differential-algebraic equations of high index, overdetermined regularization, numerical integration.

Often the modeling of dynamical processes, e.g., control problems or path following problems in multibody systems, leads to model equations in form of differential-algebraic equations of high index, i.e., differentiation index larger than two. Those high index problems contain hidden constraints which lead to instabilities, convergence problems, or inconsistencies in the direct numerical integration of these model equations.

In this talks we will discuss the efficient and robust numerical simulation of dynamical systems modeled with differential-algebraic equations of high index. We will present an approach which mainly consists in two steps. The first step consists in a remodeling of the dynamical system towards an overdetermined set of differential-algebraic equations. The obtained overdetermined formulation satisfies the requirements for a regularization and, in particular, is equivalent to the original model equations in the sense that both have the same solution set. The second step in the approach is the subsequent robust and efficient numerical integration of the regularized overdetermined formulation with adapted discretization methods. For this numerical integration we present the software package QUALIDAES which is suited for the direct application to overdetermined differential-algebraic equations arising form the previous discussed remodeling.

The applicability of the proposed approach and, in particular of QUALIDAES, for the numerical treatment of model equations with a high index will be demonstrated on several examples. Furthermore, a comparison to other solvers will be provided.

Multiphase flow computation at high Reynolds with anisotropic adaptive meshing and stabilized FE Solver

Thierry Coupez, Elie Hachem, Luisa Silva and Hugues Digonnet

Author Keywords: multiphase flow, fluid structure, stabilised finite element, anisotropic mesh adaptivity, immersed volume, level set.

Multiphase flows at high-Reynolds number are appearing in a wide range of important physical phenomena. The development of efficient methods to simulate large scale phenomenon as free surface fluid flow in large channel, hydraulic jump, breaking waves, floating bodies, fluid structure interactions and also precise physical flow as a system of bubble rising in a liquid using a unique approach is among the emerging computational challenges. Large scale turbulent regime remains a real challenge in Computational Fluid Dynamics (CFD) and there still few results nor tentative simulations for multiphase turbulent fluid dynamics. At an intermediate physical scale, by considering few isolated bubbles, it is possible to afford for the exact modeling by solving the Navier-Stokes equation in a multiphase despite the strong ratio of the density and the viscosity between the air and the liquid phases This contribution is a step forward to a unique computational framework for multiphase flow ranging from the bubbles and droplets dynamics to breaking waves and large scale hydraulic applications. The first ingredient of the proposed approach is a simple regularization by means of averaging the matter parameters through an interface of a given thickness. The second ingredient is the exhaustive use of an anisotropic mesh adaptation based on a posteriori error estimation that produces highly stretched elements. It au-

tomatically captures the interfaces helping to reduce the thickness providing the desired sharpness. This approach seems to be mature enough to offer very new possibilities in term of numerical simulation of complex multiscale physical phenomena as breaking waves, hydraulic jump and micro-fluidic dynamics, at a good level of accuracy. Direct numerical simulation for multiphase flows, are using a Stabilized Finite Element Flow solver based on Variationnal Multiscale Framework [1], a variant of the level set method [2], anisotropic mesh adaptation [3,4] and a global monolithic framework already used in FIS applications [5]

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Multiphysics and multiscale models for the simulation of filtration processes

Dimitar Iliev, Oleg Iliev, Ralf Kirsch, Zahra Lakdawala[137], Andro Mikelić[138] and Galina Printsypar[139]

The cleaning of fluids by filtering devices is a very important topic in many fields of application (civil engineering, automotive industry, biomedical sector etc.). The optimization of the design of such elements is a non-trivial task such that a purely empirical approach using real-world prototypes can become very time-consuming and costly. Computer-aided engineering (CAE) using specialized numerical simulation of filtration has proven to be capable to reduce the developmental time and/or increase the quality of the filtering device.

The mathematical modeling of filtration is a great challenge, too: The filtering process is by nature complex, involving several physical phenomena occurring at very different scales in both time and space. A starting point is the fluid flow through the housing and the filtering (porous) medium. Among others, the flow field is influenced by the geometrical shape of the housing and the porous medium. For deformable porous media, the pressure distribution in the fluid interacts with the shape of the medium such that a coupled description of this interaction is needed. This involves suitable

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modeling of the so-called poroelastic behaviour which differs significantly from classical mechanics of solids. Furthermore, the deposition of dirt particles in the filtering medium is heavily influenced by the velocity field of the fluid. On the other hand, the local permeability of the medium is directly related to the distribution of deposited dust. This means that the capturing of the particles on the micro-scale is interacting with the flow field on the macroscopic scale of the housing.

In this talk, we will present and discuss mathematical models that allow for the description of these coupled problems, together with the corresponding numerical and algorithmic approaches. The effectiveness of these methods will be illustrated by numerical case studies.

Simulation Issues for Nanoelectronic Coupled Problems

Automatic parametric model order reduction using an a posteriori output error bound

Lihong Feng, Peter Benner and Athanasios C. Antoulas

Author Keywords: Parametric model order reduction, Parametrized systems, Coupled systems, Error bound.

Abstract

Parametric model order reduction (PMOR) is an advanced model order reduction (MOR) technique for reduced order modelling of parametrized systems, e.g. micro- and nano-electrical(-mechanical) systems with geometrical, physical variations; and also coupled micro-and nano-electro-thermal problems, where the coupling terms are treated as parameters. Through PMOR, the parameters are preserved in the reduced models as symbolic quantities. The goal is that a single reduced model is accurate for all possible variations of the parameters.

We propose an a posteriori output error bound for reduced order models of linear parametrized systems. The proposed output error bound provides a way of automatically generating reliable reduced models computed by, e.g. the Krylov subspace based PMOR methods, which is desired in design automation for circuits and MEMS. Although Krylov subspace based MOR methods have been integrated into some simulation tools, the reduced model cannot be guaranteed to satisfy the required accuracy due to the lack of

a robust error bound. We are making the design automation reliable by proposing an a posteriori output error bound.

The European Project nanoCOPS for Nanoelectronic Coupled Problems Solutions

Rick Janssen, Jan ter Maten, Caren Tischendorf[140]

Abstract

The project nanoCOPS [1] is a collaborative research project within the FP7-ICT research program funded by the European Union. The consortium comprises experts in mathematics and electrical engineering from seven universities (BU Wuppertal, HU Berlin, Brno UT, TU Darmstadt, FH O Hagenberg, U Greifswald, KU Leuven), one research institute (MPI Magdeburg), two industrial partners (NXP Semiconductors Netherlands, ON Semiconductor Belgium) and two SMEs (MAGWEL, ACCO Semiconductor).

We present an overview of the project subjects addressing the *bottlenecks*

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in the currently-available infrastructure for nanoelectronic design and simulation. In particular, we discuss the issues of an electro-thermal-stress coupled simulation for Power-MOS device design and of simulation approaches for transceiver designs at high carrier frequencies and baseband waveforms such as OFDM (Orthogonal Frequency Division Multiplex).

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Dynamic Coupled Electromagnetic Field Circuit Simulation

Caren Tischendorf

Author Keywords: circuit simulation, electromagnetic field simulation, coupled problems, differential-algebraic equations, Maxwell equations, hybrid linear solver.

We discuss a wholistic circuit simulation approach coupling lumped models with 3D field models described by full Maxwell's equations in a potential formulation. We consider a simulation approach that discretizes the corresponding partial differential algebraic system (PDAE) first in space using the finite integration technique. We discuss an efficent solving of the resulting high-dimensional differential-algebraic system. In particular, we address the need of a circuit network parser generating a stable DAE formulation and allowing a fast function evaluation as well as the advances of a modular implementation of integration methods, nonlinear solvers and linear solvers. Finally, we present a structurally adapted hybrid linear solver combining direct and iterative methods.

Fast and Reliable Simulations of the Heating of Bond Wires

David Duque and Sebastian Schöps

Abstract

The ever tightening specifications imposed on modern integrated circuits (ICs) by the semiconductor roadmap demand the manufacturing of more energy-efficient chips which are constantly smaller in size. Typically, bond wires are used to establish electrical connection between the chip and the lead frame or pins during device assembly. These wires are heated due to Joule effect and their temperature increases substantially. If the wires cannot properly dissipate this excess of energy, then permanent damage will occur to the wirebonds and surrounding material. This current-induced damage is commonly recognised as fused bond wires. Hence, fusing or melting of wirebonds can be identified as one increasing potential source of failure in IC devices.

In this paper, we present an extended analytic formulation for the determination of the temperature distribution along a bond-wire within a package, and thus extract the maximum allowable current. The closed-form formula obtained involves the essential physical parameters that define a package, i.e., moulding compound material and dimensions, bond-wire characteristics, etc., by using an appropriate set of heat transfer boundary conditions (BCs). This is very important if one wants to quickly study the influence of (randomly distributed) parameter variations on the current capacity of the wire by means of uncertainty quantification (UQ) methods.Several simplistic analytic formulations for the estimation of current capacities in bond-wires

have already been proposed [1, 2, 3, 4, 5]. Nonetheless, in their attempt to oversimplify the resulting partial differential equation (PDE) and associated BCs so as to cope with the non-linearities introduced by the thermal variations of the wire parameters, the resulting formulations end up lacking the variables that define a package as a geometrical shape; furthermore, they often neglect the influence of the finite thermal capacitance of the lead in the wire temperature distribution. In this paper, we shall address these typical deficiencies while providing a thorough assessment of our model by means of computer simulations.

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Multiphsyics simulation in electrical engineering

Nonlinear model reduction for simulation of coupled systems

Johanna Kerler and Tatjana Stykel [141]

Abstract

Recent technological and industrial developments have caused a considerable interest in the study of dynamical processes modeled by coupled systems of ordinary differential equations, differential-algebraic equations and partial differential equations. Application areas of coupled systems include circuit-device simulation and micro-electro-mechanical systems. The dynamical behavior of such systems is determined by different interconnected subsystems that are usually governed by entirely different physical laws and often act in different time and space scales. In this talk, we discuss the simulation of coupled nonlinear systems using dynamic iteration combined with model order reduction. We study the convergence of this approach, derive error estimates for approximate solutions and present methods to efficiently calculate the error estimates. Numerical examples will demonstrate the properties of the presented integration method.

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Exponential integration methods for water transportation networks

Lennart Jansen

Author Keywords: Exponential integration methods, Water transportation networks, Differential algebraic equation

Abstract

We consider a partial differential algebraic equation (PDAE) model describing water transportation networks including pipes, tanks, pumps and valves. We focus onto the water transport over long distances with a laminar flow model description for the pipes. It is well known that a proper space discretization should guarantee volume conservation. Sadly the differential algebraic equations (DAEs), which result from a volume preserving space discretization, have rather complex structures, i.e. the calculation of the inherent ordinary differential equation (ODE) may be expensive. In particular the midpoint rule yields a semi-linear DAE with index 2, even if we consider a water transportation networks including only pipes. But, for a efficient numerical simulation of the space discretized PDAE, one is interested in space discretizations that result in a DAE with a low index and a profitable structure.

We present here a space discretization resulting in a semi-explicit index 1 DAE. In particular it is possible to extract the inherent ODE of the system by little effort. We will show that one has to exploit the network topology in order to achieve this goal. The special structure of the inherent ODE enables us to apply exponential integration methods and model order reduction

techniques. In this talk we will demonstrate how the exponential integration methods accelerate the simulation of water transportation networks.

Model Order Reduction for Mutlirate ODE-Solvers in Multiphysics Application

Christoph Hachtel, Michael Günther and Andreas Bartel [142]

Abstract

In general, the modelling of a multiphysical setting leads to a coupled system with largely differing dynamical behaviour. Possibly after a semi-discretization of the spatial variables, these models are often given by coupled systems of ODEs. Now, the most stiff part suggests which type of time domain method should be applied. Furthermore the most active part, i.e., the part with the highest frequencies, determines the step size to be used.

Multirate ODE-solvers allow us to use different step sizes for each subsystems. The use of inherent step sizes for the subsystems with different dynamical behaviour gives us potential to enhance the numerical efficiency (the performance concerning computation time). The crucial part of a multirate solver is the coupling of the different scales, i.e., the computation of the coupling variables. There are several approaches define the coupling (e.g. [1], [2], [3]). Often the physics of the underlying systems justifies the usage of a certain coupling type. Although one saves computation time due to larger step sizes for latent components (macrostep), usually a large and stiff system remains to be solved in each macrostep.

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In the last years, model order reduction has been developped to a reliable technique to solve high dimensional systems of differential equations efficiently [4]. Until now there has been no work on combining model order reduction with multirate ODE-solvers. In this talk we present related ideas and concepts of the reductionmultirate methods and give first numerical results for a multiphysics example.

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Eddy current model for non-destructive testing of electrically conducting materials with cylindrical symmetry

Valentina Koliskina, Andrei Kolyshkin, Olev Martens, Rauno Gordon, Raul Land and Andrei Pokatilov

Author Keywords: eddy current testing, semi-analytical method, change in impedance, numerical simulation.

Eddy current method is widely used in practice for quality testing of conducting materials (examples include determination of electrical conductivity, thickness of metal coatings, identification of flaws in a conducting medium). All the above mentioned problems are inverse problems. In order to solve an inverse problem one has to have a reliable and fast method for solution of a direct problem. In the present paper we propose a semi-analytical method for solution of direct eddy current problems for the case of a conducting medium of finite size. The method is applied to several eddy current problems with cylindrical symmetry. The following problem is analyzed in detail. Consider a coil with alternating current located above a conducting medium in the form of a circular cylinder (such a model can be used for design of coin validators which are based on the estimation of electrical conductivity of a coin). We assume that the electromagnetic field is exactly zero at a sufficiently large distance from the coil (the distance can be chosen on the basis of the required accuracy of the solution). The solution is constructed using the method of separation of variables which includes

two steps where numerical calculations are necessary: (a) computation of complex eigenvalues without good initial guess for the roots and (b) solution of a system of linear algebraic equations. Computations of the change in impedance of the coil for different frequencies with the semi-analytical method are in good agreement with experimental data and results of numerical simulation with finite element method. Solution of other problems with cylindrical symmetry is also presented (a flaw in the form of a circular cylinder in a conducting half-space or a plate) . Such models can be used for the analysis of quality of spot welding (in case of a volumetric flaw) and estimation of the effect of corrosion (for surface flaws).

Current Challenges in Computational Finance

Finite difference methods with third level algebra

Giacomo Pietronero

Author Keywords: finite difference methods, operator methods, quantitative finance, computational finance, BLAS, GPU, Crank-Nicolson.

Abstract

Finite difference methods (FDM) have been developed and optimized in a technology context that is no longer current. When FDMs affirmed themselves as a standard it used to be that memory was a scarce resource and that algorithms were either memory or compute bound. As a consequence traditional FDMs have been designed to minimize the number of operations and the memory footprint to the detriment of accuracy. The potential of computers in terms of floating point operations per seconds (FLOPS) and memory available increased dramatically over the last years offering an opportunity for a rethink of the way finite difference methods are implemented. Nowadays only a small class of algorithms are able to exploit the computational power of modern hardware. Most algorithms, including the (sparse) matrix-vector multiplication (BLAS 2) that is a cornerstone of traditional finite difference methods, are bounded by the number of memory reads and therefore are unable to exploit the computational power of parallel computing. To highlight these limitations we analyse the performance of FDMs on GPUs and compare it to a framework proposed by Albanese that is based on matrix multiplication (BLAS 3) and aims at retaining modelling flexibility while being a compute bound algorithm.

Portfolio simulations for the "mega-models"

Claudio Albanese and Giacomo Pietronero

Author Keywords: Quantitative finance, computational finance, Portfolio simulation, derivatives, CVA, DVA, FVA, parallel computing, grid computing.

Abstract

In the aftermath of the crisis, the credit and the funding components of the derivatives business have been attracting much attention. To quantify these effects, banks need to carry out large Monte Carlo simulations of their derivatives portfolio. Typical portfolios entail hundreds of thousands of derivative transactions. Simulations involve hundreds of time steps over horizons of about 50 years. The traditional modelling approach implemented by most banks is transaction-centric. Individual trades are valued using the model deemed most appropriate even if this gives rise to inconsistencies between trades. The calibration process to market-data is also transaction specific. Portfolio simulations require a radically different and more holistic approach, whereby global models are used for scenario generation and portfolio valuation. Also, in memory implementations on large memory supercomputers are more effective than algorithms distributed on large clusters. The talk dwells on how mathematics can be optimized to large memory boards in order to marginalize both the network and the memory bottlenecks.

Speeding Algebraic Pricing Methods using Matrix Operations on GPU

Paolo Regondi, Claudio Albanese and Mohammad Zubair

Author Keywords: BLAS, CUDA, PDE pricing methods.

PDE pricing methods such as backward and forward induction are typically implemented as unconditionally marginally stable algorithms in double precision for individual transactions.

In this paper, we reconsider this strategy and argue that optimal GPU implementations should be based on a quite different strategy involving higher level BLAS routines. We argue that it is advantageous to use conditionally strongly stable algorithms in single precision and to price concurrently sub-portfolios of similar transactions.

To support these operator algebraic methods, we propose some BLAS extensions. CUDA implementations of our extensions turn out to be significantly faster than implementations based on standard CUBLAS.

Probabilistic interpretation of finite difference methods

Sebastian Del Bano Rollin, Claudio Albanese and Giacomo Pietronero

Author Keywords: Mathematical finance, Levy processes, Finite different methods, Implicit methods, Option pricing, Subordinator, Gamma process.

Implicit finite difference schemes have an intriguing probabilistic interpretation in terms of Bochner subordination. In particular we show that, for a generic Levy process, the transition semi-group that is the result of an implicit scheme approximation can be also obtained using a Gamma process to subordinate the original process.

In this talk we also discuss how the strong convergence properties of implicit methods are related to this property.

Poster Presentation

Model Design of ERP Architecture based on SAP HANA Security

Roumiana Antonova, Galia Novakova, Dimitar Birov, Kamen Spassov, Dobrinka Stefanova and Ingo Bremer [143]
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Abstract

Now that large-scale companies and startups have similar opportunities to do business on the Cloud, the number of cloud software vendors is expected to become immense. On the other hand, drastic cost savings and low startup costs allow us to expect more and more data to be outsourced to the Cloud in the coming years. This inevitably brings up the question that we discuss in the present paper: is the Cloud industry as reliable as we expect it to be?

Security on the Cloud is one of the Cloud-related topics that everyone wants to talk about... yet, no one wants to think about. Cloud companies want us to believe security on the Cloud is granted. But is it so? Companies do invest a lot in building strong security infrastructures. But is it enough for us to assume our data is at least as safe on the Cloud as in a good old on-premise system?

Our data being on the Cloud means our data are 24/7 accessible online in a shared system, accessible over the Internet from different devices from any spot in the World. This comes into contrast with on-premise systems,

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where data is physically and virtually isolated, and Web-based access is usually restricted. So, what makes us leave this well-explored security domain (which also has numerous security holes), and go for the potentially far more vulnerable Cloud world? Well, the numerous advantages of cloud computing do: lower TCO, connectivity, mobile access, and so on. This doesn't mean that we care about security any less. On the contrary, if data is the world's new currency, we want ours to be securely stored on the Cloud.

In the present paper we present a case study dealing with security on SAP HANA Cloud Platform. The discussed platform is SAP's platform-as-a-service (PaaS). It provides a platform where application developers can run their cloud software, and provide it to end customers. It gives a number of advantages to its users. This platform provides a set of services that developers can use to provide easily complex functionality to users. Besides its commercial program for customers and partners, it comes with a free developer program for all application developers who are willing to try out SAP HANA Cloud Platform. Developers need to register on SAP Community Network (SCN) and accept the end user license agreement of that platform. From then on, they can deploy on SAP HANA Cloud, and access many of the benefits provided to paying customers, as long as they do not use it for commercial applications.

The present platform allows application developers to adopt a widespread community standard for application development: Java Enterprise Edition (Java EE). In this way, application developers could easily and rapidly create brand new or port existing Java EE applications to the Cloud. SAP HANA Cloud Platform also provides a set of developer tools for the most popular Java development environment - Eclipse. Cloud. SAP HANA Cloud Platform allows application developers to secure their applications in miscellaneous ways.

To be able to incorporate an existing identity management infrastructure on the proposed platform, an administrator needs to configure trust settings both on the Cloud and on the identity provider. This means one needs to set up SAP HANA Cloud Platform to trust the identity provider, and the identity provider to trust SAP HANA Cloud Platform.

SAP ID Service is an out-of-the box solution that you can use if you don't have a corporate identity management infrastructure. It is the default identity provider for the given platform, and you can use it without having to configure SSO and identity federation. The discussed platform allows you to manage the access to your applications based on Java EE security roles. This approach is called *declarative authentication* because you only declare what you need to protect and how.

So that, in the case study presented in this paper the authors show that it is simple and powerful, very fast and relies on the built-in security implementation in SAP HANA Cloud Platform. If you want to have fine-grained control over access to your application's resources, and still take advantage of that platform's role management, you can use this platform's security API to implement programmatic authentication. Besides, the paper presents also a comparison between other similar systems.

Key words: Modeling, Design, ERP Architecture, SAP HANA, Security

Mathematical description of timing belts motion in the process of coupling

Grzegorz Domek and Marian Dudziak

Author keywords: gears, timing belts, couplin process

Abstract

Although the timing belts are manufactured for over 60 years were never adequately describe the movement of the belt in the process of conjugation. Willis principle perfectly describes the collaboration of two cylindrical gear wheels, dominated the thinking of designers, who all the time assumed approximately the phenomena in the transmission of a timing belt. Sought-ray market, and above all an anchor reference plane. It was established that the plane is a the carrier layer. One of the basic parameters of the transmission belt- the pitch, is measured on of this plane. Amount has not been established so far description of belt movement relative to the wheels. Presented at work approximate description of the motion of the pendulum with variable attachment point is the nearest real phenomena. This description allows to re-plot the geometrical form of the tooth belt and wheels. Allows to develop the optimum tooth shape for the coupling process.

New approach to description of friction in the gear with timing belt

Grzegorz Domek and Marian Dudziak

Author keywords: friction, timing belts, mechanical gears

Abstract

Friction in the belt gears are known and described already many years. This does not include the transmission of a gears with timing belt. Until now, many authors still believe that there is only shaped coupling. Thorough analysis shows that is depending on the type and size of belts and circumferential force. Large part of the torque in such gear is transmitted via frictional engagement. This paper attempts to mathematically description of this part of the coupling, through the development of Coulombs model and by analyzing the stress and strain at the timing belt.

Influence diagrams to aid decision making

Winston Sweatman, Haydn Cooper, Philip Kilby and Graeme Wake

Author keywords: mathematics in industry study group, influence diagrams, decision making tools

Abstract

Influence diagrams are a tool for decision making. They are formed by a network of linked events. The exploration, analysis and interpretation of these structures was the subject of a project at the mathematics-and-statistics-in-industry study group at RMIT University in Melbourne in 2010 (MISG 2010).

In this poster we illustrate some of the results arising from that investigation. Transmission of influence can take place through multiple events and the links between these events. Simple models can be understood as dynamical systems which evolve as the effects of influence make their way through the diagram. Computer simulation is a useful tool, readily providing illustration to aid understanding and interpretation of the process.

Stochastic Butler-Volmer dynamics in modelling lithium-ion battery electrodes

Chang Wang

Author Keywords: Lithium-ion batteries, Butler-Volmer kinetics, discrete-continuum model, asymptotic analysis, dynamical system.

Abstract

The work originates from my PhD project in modelling electrode current in lithium-ion batteries by incorporating the Butler-Volmer equation with a logarithmic double well potential. First we study a Butler-Volmer style model to describe electrode kinetics when controlled by a time-varying external potential. A matched asymptotics analysis reveals a delayed bifurcation when the controlling parameter passes through the critical values for the bifurcation plot. To see would the bifurcation be altered when fluctuations due to thermal noise are taken into account, we study a stochastic model. Some similar works used a Fokker-Plank type of equation. Instead we derive a discrete-continuum model from the microscopic one-step process which implies the Fokker-Planck type of equation in its continuum limit but also suggests a regime where the discrete nature is essential and the Fokker-Planck equation does not give an accurate description. We are able to simplify the discrete-continuum model and quantify the effect of thermal noise. We hope that identifying the essential dynamics would assist building second effects into the model.

Axial load distribution of contact stresses in involute splined connections

Jacek Kroczak and Marian Dudziak

Author Keywords: involute splined connection, form deviation, contact stress.

Splined connections are direct joints and are used to align and transfer the torque. In mechanical engineering the following modifications of splines are used: straight-sided spline, involute spline, and serrations. Involute splined connections are more and more used, especially in aircraft and automotive industry, because in comparison with other splined connections these connections are characterized by: high strength of spline, low stress concentrations, radial alignment of mating elements, and self-acting coaxial align of the hub and the shaft under loading. After machining and heat treatment of involute splines, one can not obtain a perfect external or internal involute spline. There will always be some form deviations. These deviations affect the maximum material condition and hence the fit of connection. The form deviations are complex and occur on each flank of space and tooth. The most important spline deviations are: pitch deviation, profile deviation, and lead deviation. The authors have stated that there is a lack of exact information on a load distribution in splined connections with different types of manufacturing errors. Hence, the analysis of the influence of a pitch deviation on the axial distribution of contact stresses is presented.

Minisymposium: Mathematics in Nanotechnology

Dynamics of bacterial aggregates in microflows

Ana Carpio, David Rodriguez and Baldvin Einarsson

Author Keywords: Biosensors, MEMS, biofilms, aggregation, microflows, multiscale, streamers.

Abstract

Biofilms are bacterial aggregates that grow on moist surfaces. Stable biofilms formed naturally on the walls of conducts may serve as biosensors, providing information on the status of microsystems (MEMS) without disrupting them. However, uncontrolled biofilm growth may largely disrupt the environment they develop in, increasing the drag and clogging the tubes. To ensure controlled biofilm expansion we need to understand the effect of external variables on their structure. We formulate a hybrid model for the computational study of biofilms growing in laminar microflows. Biomass evolves according to stochastic rules for adhesion, erosion, motion and cell division, informed by numerical approximations of the flow and concentration fields at each stage. The model is tested studying the formation of streamers in three dimensional corner flows, gaining some insight on the effect of external variables on their structure.

Dynamics of optically injected currents in carbon nanotubes

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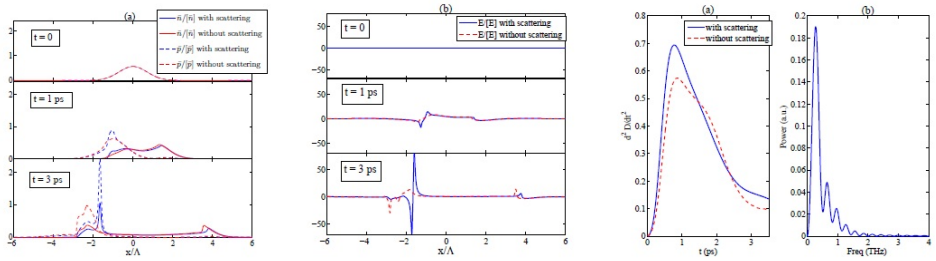
Abstract

Optical manipulation of carriers in solids is an interesting problem for fundamental and applied physics. By an interference of single and two-photon transitions one can inject optically currents in semiconductors and semiconductor nanostructures. Recently, current injection was reported for graphene and carbon nanotubes. Dynamics of the injected currents is an interesting problem since it can provide a valuable information about interactions in the system. In addition, the spectrum or radiation emitted by time-dependent currents is of interest. Here we consider theoretically dynamics of currents optically injected in carbon nanotubes. We assume that the main effect on the dynamics is due to the space-charge forces. We calculate time evolution of the dipole moment and spectrum of the corresponding radiation, which is in the frequency range of the order of 1 THz for typical system parameters.


(a)
$n/|n|$ with scattering
$n/|n|$ without scattering
$p/|p|$ with scattering
$p/|p|$ without scattering
t = 0
t = 1 ps
t = 3 ps
x/Λ
(b)
E/|E| with scattering
E/|E| without scattering
t = 0
t = 1 ps
t = 3 ps
x/Λ
(a)
with scattering
without scattering
n^2 (cm^{-3})
t (ps)
(b)
Power (a.u.)
Freq (THz)

Mathematical model for the melting of a nano-thin film

Francesc Font Martinez and Tim Myers

Author Keywords:nano-thin film, phase-change, Stefan problem, hyperbolic PDE

When the size of a physical system is of the same order of magnitude of the mean free path of the heat carriers the Fourier law breaks down. This can be resolved by adding a lag term in the expression for the heat flux, accounting for the delay between an applied temperature gradient and its influence on the heat flux. Combining the new expression for the flux with the energy equation leads to a hyperbolic heat conduction equation. Indeed, the mathematical model describing the phase change of such systems will be remarkably different from the standard Stefan problem. In this talk I give an overview of the recent work done on this topic by our group.

Boundary layer analysis and heat transfer of a nanofluid

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Abstract

Efficient heat removal is one of the most important problems currently facing industry. For example the high process density circuit boards used in the telecommunications industry means that companies expend more than 50% of their electricity on cooling systems. Certain high power electronic devices require heat removal rates of the order $2000W/cm^2$. Air cooling methods are limited to around $100W/cm^2$. Consequently, there is a vast amount of research into novel methods for cooling. One of the forerunners in this race is the nanofluid (a fluid containing nanoparticles).

There exist numerous experiments demonstrating nanofluids to have remarkable proper- ties. However, there has been much controversy in the literature with discrepancies between results concerning the heat transfer and thermal conductivity of nanofluids. In this talk we first present a model for the thermal conductivity of a nanofluid and show that it compares favourably to experimental data. We then carry out an analysis of a nanofluid flowing past a flat plate to show that, contrary to numerous experiments, the heat transfer coefficient actually decreases with particle concentration. We also explain some of the reasons for the results, both numerical and theoretical, that have come to the opposite conclusion.

Ab-initio based Kinetic and Transport Models

Robust and Efficient Tandem Thin Film Sillicon Solar Cells

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Author Keywords: Multi-objective optimization, Single-objective optimization, Sensitivity Analysis, Robustness Analysis, Identifiability Analysis, Exact Maxwell Simulation, Photonic Monte Carlo Simulation, Transparent Conductive Oxide materials, Back Reflectors.

In this research work we present and deeply analyze an optical model for tandem thin film sillicon solar cells, using different Transparent Conductive Oxide materials, different Back Reflectors, varying the doping dosage and the materials roughness. The Analysis is composed of five distinct steps: i) Sensitivity Analyisis, to establish every parameter influence and to understand the contribute it has on the output; ii) single objective optimization, to fully optimize the quantum efficiency of solar cell devices; iii) multi objective optimization, to balance quantum efficiency and cost savings and, inter alia, to obtain robust designs; iv) Robustness analysis, local, global and glocal, that assigns to each optimal designs robustness indexes; v) data-based identifiability analysis of the model, here used to infer functional relationships among notable points sets. The optical model implemented is a fine-balanced combination of exact Maxwell simulation, applied to capture light scattering effects in nano-textured interfaces, and a photonic Monte Carlo simulation, which statistically evaluates coherent and scattered light photon absorption in the layers. We applied our methodology to different cells topologies and different materials, obtaining remarkable improvement and demonstrating the solidity and flexibility of the methods used.

Should molecular lattices always be the most densely packed ?

Fabrizio Cleri, Guillaume Copie, Cristhope Krzeminski and Bruno Grandidier

Author Keywords: molecular self-assembly, molecular simulation, semiconductor surfaces, total energy methods, statistical thermodynamics, global optimization.

High-density packing in organic crystal is usually associated with an increase of the coordination between molecules, since the early formulations of molecular symmetry arguments by Kitaigorodski in the late 50s. We contend the validity of this concept for two-dimensional molecular networks self-assembled on solid semiconductor surfaces, by using a combination of scanning tunneling microscopy experiments and multi-scale computer simulations. We study the phase transitions between different polymorphs and we demonstrate that, contrary to simple intuition, the structure with the lowest packing density may correspond indeed to the highest coordination. The subtle competition between intermolecular and surface dispersion forces (often ignored in the discussion of molecular symmetry) is at the origin of such a counter-intuitive result. Having the lowest free energy, such low-density structures spread out macroscopically as the most stable polymorphs over a wide range of molecular concentrations.

Theoretical structure prediction

Stefan Goedecker

Author Keywords: structure prediction, density functional theory, global optimization.

Atomistic systems can adopt a huge number of metastable configurations with quite different properties. Theoretical structure prediction methods can find such low energy configurations including the lowest energy ground state and it is widely believed that they will play an increasingly important role in materials discovery. I will briefly review the fundamental challenges of theoretical structure prediction as well as some common approaches to this challenging task, I will in particular describe the basic principles of the minima hopping method and I will give illustrative examples of structures found by this method. These examples will include clusters, crystaline strucures and surfaces.

Plenary Talks

Mathematics applied to Analog Circuit Simulation

Pascal Bolcato (Mentor Graphics Corporation)

Abstract

An Analog Circuit Simulator is a mandatory tool in automated design of electronic integrated circuits. It is used during the design and verification phases of Analog IP blocks.

It computes the behavior of electronic circuits from their topological and component descriptions. An analog simulator, first, build a system of equations. Then it solves it in order to calculate the circuit response according to specified stimuli. Depending on the analyses, the systems to be solved by the simulator are linear or non-linear, real or complex, algebraic or differential. The number of equations/unknowns is proportional to the number of nodes in the circuit and can easily reach several tens of million. As it directly affects the circuit designer productivity, simulator performance and scalability is of paramount importance and is an endless challenge. That is why modern circuit simulators use state-of-the-art mathematical techniques in the area non-linear algebraic solvers, DAEs time integration, direct and iterative linear solvers, preconditioning techniques, graph partitioning, ... During this presentation, the algorithms used in transient Analysis and Steady-State analysis are monitored with a special emphasis on the linear solver part. And, as execution performance is an important concern, some stress is put on parallelization of the corresponding algorithms and their software implementations.

Design of silicon based integrated optical devices using the finite element method

Paolo Pintus

Author Keywords:Maxwell's equations, finite element method, waveguide mode solver, anisotropic waveguide, magneto-optical waveguide.

Abstract

Among the components needed in photonic integrated circuits, dielectric waveguides and small footprint ring resonators play a key role for many applications and require sophisticated electromagnetic analysis and design. In this work, we present an accurate vectorial mode solver based on the finite element method. Considering a general nonreciprocal permittivity tensor, the proposed method allows us to investigate important cases of practical interest. To compute the electromagnetic modes, the Rayleigh-Ritz functional is derived for the non-self adjoint case, it is discretized using the node elements and the penalty function is added to remove the spurious solutions. Although the use of the penalty function is well known for the waveguide problem, it has been introduced for the first time (to the best of our knowledge) in the ring resonator modal analysis. The resulting quadratic eigenvalue problem is linearized and solved in terms of the propagation constant for a given frequency (i.e., $\gamma-$formulation). Unlike the earlier developed mode solvers, our approach allows us to precisely compute both forward and backward propagating modes in the nonreciprocal case. Moreover, it

avoids time-consuming iterations and preserves matrix sparsity, ensuring high accuracy and computational efficiency.

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