BOOK OF ABSTRACTS

Workshop on Industrial and Applied Mathematics 2016

Hamburg, 31.08. - 02.09.2016

WIAM 16

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1 Talks

1.1 Session THU-1 (Thu, 09:00 – 10:40, lecture hall H1)

1.1.1 Laurent Stainier, Thomas Heuzé, Jorge De Anda Salazar

Development of algorithmic strategies for numerical simulation of coupled mechanical-diffusion problems

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Abstract

The aim of the research is the exploration of novel algorithms strategies for numerical simulation of non-linear strongly coupled mechanics-diffusion problems. The former is based on a proposed variational formulation approach which provides a natural framework for coupled problems, with numerical benefits such as efficiency, flexibility and robustness in algorithms overcoming classical results. Through a variational formulation, the solution for a mechanics-diffusion problem can be stated as an optimization process.

A description for the development and numerical implementation of a variational formulation for transient-diffusion boundary-value problem will be presented. In specific, a non-linear model and its linearized version are solved for a "concentration-shock" problem. The numerical results obtained are compared against classical methods derived from a weak formulation. The spatial discretization is done using a finite element approach in all cases. Temporally, the Crank-Nicolson and an Implicit discretization are used for the weak derived schemes, while for the variational formulation an implicit-explicit is selected.

The goal of the variational formulation for transient diffusion problems is in our interest since it settles a path to follow for the modeling and resolution of coupled problems. Mechanical-diffusion problems, provide a wide range of applications among many fields, from reactive flows in solids to tissue reconstruction by means of hydrogels, among others.

Keywords
variational formulation, coupled problems, discrete variational formulation, irreversible processes

1.1.2 Thomas Frenzel, Alexander Mielke

Evolutionary Γ-convergence for a delamination model

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Abstract

We consider a (discrete) parameter-dependent delamination problem, formulated as a (classical) gradient flow. The formulation of parameter-dependent parabolic equations in terms of gradient flows gives a powerful framework developed in [3, 1, 2] for the limit passage of evolutionary systems. A gradient flow is generated by a gradient system $(X, \mathcal{E}_\varepsilon, \mathcal{R}_\varepsilon)$, where X is the state space, $\mathcal{E}_\varepsilon$ is the energy functional and $\mathcal{R}_\varepsilon$ is the dissipation potential. Then the gradient flow can be stated via the energy-dissipation-balance

$$\mathcal{E}_\varepsilon(T, u(T)) + \int_0^T \mathcal{R}(\dot{u}) + \mathcal{R}^*(-\mathrm{D}\mathcal{E}_\varepsilon(t,u))\mathrm{d}t \leq \mathcal{E}_\varepsilon(0, u(0)) + \int_0^T \partial_t \mathcal{E}_\varepsilon(t,u)\mathrm{d}t. \tag{EDP}$$

This formulation is the starting point to apply variational techniques.

The breaking of the bonds between particles, i.e., the delamination is described via a non-convex potential which generates a micro-structure acting on a different scale. Moreover, it's the limit of the micro-structure that leads to non-uniqueness of solutions to the limit equation and destroys the gradient structure.

References

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[3] E. Sandier and S. Serfaty. Gamma-convergence of gradient flows with applications to Ginzburg-Landau. *Comm. Pure Appl. Math.*, LVII:1627–1672, 2004.

Keywords

parabolic semi-linear PDE, gradient flow, evolutionary Γ-convergence, multiscale, delamination

1.1.3 Mauricio Garcia-Vergara, Guillaume Demésy, Frederic Zolla

Transient regime in highly dispersive media

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Abstract

In a non dispersive medium, an arbitrary pulse would propagate unaltered. In a frequency dispersive material, however, the pulse is modified as it propagates. The study of the propagation of electromagnetic fields (such as optical pulses) through dielectric media, possibly exhibiting both dispersion and absorption, goes back to the early 1900's papers by Sommerfeld and Brillouin. A significant contribution to the study of this phenomenon has been done by Oughston in the 70's , by using complex and asymptotic analysis techniques. Nevertheless some well established concepts in the case of non dispersive media need to be revisited.

Our analysis consist in a detailed development of the theoretical aspects together with rigorous numerical simulations, of pulsed electromagnetic radiation in a causal linear medium. We consider homogeneous and isotropic media with general, possibly extreme, dispersive and absorptive properties. In order to ensure that our analysis respects the principle of causality we have chosen a single resonance susceptibility given by a Lorentz model, keeping in mind that the features of a more complex material can be modeled using a sum of these elementary terms. At this stage of our research, we have been working on the study and numerical simulation of an electromagnetic wave packet, that propagates in single slab of extremely frequency dispersive material embedded in vacuum. The methodology used is based on temporal Fourier transformation, PDE's, and complex analysis techniques. The numerical results obtained allow us to analyze two basic concepts in electromagnetic wave propagation: The very definition of energy and the associated wave propagation velocity.

Keywords

wave propagation, energy transfer, resonance, dispersion

1.1.4 Masoud Ghaderi Zefreh[1], Florian Doster[1], Marc Hesse[2]

Fit-for-purpose Simulator for Scale Management at Production Wells

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Abstract

Pressurized underground oil/gas reaches the surface through *production wells*. Different streams of fluid from different subsurface location converge at production wells. Water is always present with the other hydrocarbons. When water from different origins with different compositions mix, the composition is usually out of equilibrium. Therefore, the mixture approaches a new equilibrium through chemical reactions. The new equilibrium is sometimes accompanied by precipitation of salts and scales. Production well damage through the occlusion of flow pathways due to precipitation of scales and salts is called *scaling*. The damage through scaling requires costly intervention and remediation strategies. To manage scaling is officially paramount to understand the process.

Numerical methods are used to study the timing and the location of scaling. However, due to highly complex and non-linear nature of chemical reactions and inherent dispersion in numerical solvers, these methods usually fail to produce reasonably accurate result at affordable computational costs. Here, we address this challenge with the set of the tools from the theory of hyperbolic PDEs. We analyse the non-linear wave structure of the underlying equations that describe the transport and the reactions of the different brine compositions.

As the first step, an analytical solution is provided for the case when two brines mix. The solution deals with the case when the Jacobin matrix and therefore the behavior of the system changes from one region to the other. This results in detached Hugoniot loci. In addition, the eigenvalues get a multiplicity more than one in a region. However, by defining one admissibility condition for shocks and another for the superposition of waves, the uniqueness of the solution can be proved.

Keywords

scaling, reactive transport, hyperbolic PDE, shock/rarefaction waves, contact discontinuity

1.2 Session THU-2.1 (Thu, 11:00 – 12:40, lecture hall H1)

1.2.1 Cleophas Kweyu, Lihong Feng, Matthias Stein, Peter Benner

Reduced Basis Method for Poisson-Boltzmann Equation

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Abstract

Reduced basis methods (RBM) aim to efficiently compute numerical solutions for parametrized PDEs in real-time and many-query scenarios by exploiting an offline/online procedure which ensures accurate approximation of the truth solution in a rapid and inexpensive manner. The Poisson-Boltzmann equation (PBE) is a nonlinear elliptic PDE that arises in biomolecular modeling and is a fundamental tool for structural biology. It is used to treat electrostatic effects of biomolecules in ionic solutions. We consider a protein molecule immersed in some electrolyte, for example a salt solution, and determine the electrostatic potential triggered by the interaction between the two dielectric materials. The kind of electrolyte considered is monovalent, in which the cations and anions dissociate in the ratio of 1 : 1. This implies that the ionic strength equals to the concentration of the ions and the source of nonlinearity is a hyperbolic sine function instead of an exponential function. Proteins are not highly charged as compared to nucleic acids and therefore, it suffices to consider the linearized PBE (LPBE) and still obtain accurate results. The ionic strength acts as a physical parameter of the LPBE, and we observe the electrostatic potential under the variations of this parameter. We discretize the LPBE with a centered finite differences scheme and the resulting parametrized linear system is of more than 1.6×10^6 degrees of freedom. We solve this full order model (FOM) by the preconditioned conjugate gradient (PCG) method with algebraic multigrid as the preconditioner at different samples of ionic strength. Zero Dirichlet boundary conditions are used to avoid the dependence of the boundary data on the parameter as well. The RBM is then applied to the high-fidelity FOM and numerical results are presented. We notice that the

RBM reduces model order to $N = 6$ at an accuracy of 10^{-9} and reduces computational time by a factor of 1244.

Keywords
reduced basis method, Poisson-Boltzmann equation, ionic strength, monovalent electrolyte, finite differences scheme, preconditioned conjugate gradient

1.2.2 Iryna Kulchytska-Ruchka[1], Jan-Eric Wurst[2]

Acceleration of FEM Computations for Induction Machines

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Abstract

Transient finite element simulations with impressed stator currents are commonly used within the virtual design process of induction machines, e.g., asynchronous machines. Long computational times are required for typical simulations to attain their stationary solution. Hence, an efficient algorithm that accelerates convergence to the steady state is developed. The method is based on performing the transient finite element analysis starting from an initial state close to the steady state. Approximation of the initial guess by means of harmonic analysis is the core of the proposed approach. Numerical results verify the effectiveness of the method.

Keywords

Induction machines, steady state, transient finite element analysis

1.2.3 Rinel Foguen Tchuendom

Uniqueness for Linear-Quadratic Mean Field Games with common noise

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Abstract

The theory of Mean Field Games (MFGs for short) is concerned with the study of asymptotic Nash equilibria for stochastic differential games with infinitely many players subject to a mean field interaction (i.e each player is affected by the other players only through a function of the empirical distribution of the system).

A Nash equilibrium constitutes a consensus (or compromise) between all the players from which no player has unilateral incentive to escape.

The purpose of this talk is to show that a common noise may restore uniqueness in mean-field games. To this end, we focus on a class of examples driven by linear dynamics and quadratic cost functions. Given these linear quadratic mean-field games, we prove existence and uniqueness of solutions in presence of common noise and construct a counterexample in absence of common noise. This illustrates the principle, already observed in dynamical systems like ODEs, that introducing an appropriate noise may restore uniqueness.

Keywords

mean-field games, common noise, restoring uniqueness

1.2.4 Bismark Owusu Tawiah

Nash equilibrium in evolutionary competitive models for crop production under external regulation

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Abstract

The object of this talk is to study the cocoa market using evolutionary game theory as a framework. The entities of this competitive model are cocoa farmers and Agro-Companies, with and without external regulation. Cocoa farmers can be skilled or not whiles Agro-Companies can either be innovative or not. Generally the economy rests in a poverty-trap, where cocoa farmers are not skilled and agro-companies are not innovative. This fact suggests the need of an external agent that promotes the economy in order not to fall in a poverty trap. Therefore, an evolutionary competitive model is introduced, where an external regulator provides loans to encourage cocoa farmers to be skilled and companies to be innovative. This model includes poverty traps but also other Nash equilibria, where cocoa farmers and Agro- Companies are jointly innovative and skilled. The external regulator, in a two-phase process (loans,taxes) achieves a common wealth, with a prosperous economy, with innovative and skilled cocoa farmers.

Keywords

poverty trap, Nash equilibrium, external regulator

1.3 Session THU-2.2 (Thu, 11:00 – 12:40, lecture hall H3)

1.3.1 Mariia Dvoriashyna[1], Rodolfo Repetto[1], Jennifer H. Tweedy[2]

Aqueous Humor Flow in the Posterior Chamber of the Eye with Iridotomy

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Abstract

The posterior chamber of the eye is the region between the iris and the lens. It is connected with the anterior chamber through the pupil. Both chambers contain the aqueous humor, which is a fluid with approximately the same properties as water. The aqueous humor is produced at a constant rate in the ciliary processes, it flows in the posterior chamber, passes through the pupil into the anterior chamber and is drained at the trabecular meshwork. This slow bulk flow is very important physiologically, since the resistance to the aqueous outflow governs the intraocular pressure.

Iridotomy is a procedure in which a hole is surgically created in the iris to allow aqueous humor to flow from the posterior to the anterior chamber. It is done in cases in which there is concern that this flow might otherwise not occur freely. The choice of optimal size and location of an iridotomy is still poorly understood. The goal of the present work is to model the aqueous flow in the posterior chamber with an iridotomy and to investigate the effect of the location and size of the hole on the pressure and stress on the surrounding tissues.

We derive the shape of the posterior chamber from ultrasound images. Since its geometry is long and thin, we use lubrication theory to simplify the problem and we justify a quasi-steady approach to model miosis. In our model we treat the iridotomy as a point sink in the iris and we assume the flux through it is proportional to the pressure drop across it. To this end, we work in terms of a suitably regularised pressure and solve the problem using a finite difference method.

The results suggest that the geometry of the posterior chamber sig-

nificantly influences the pressure and flow, and in particular the height and length of the iris-lens channel and the diameter of the iridotomy. Conversely, the location of the iridotomy on the iris does not have a significant effect. During miosis, a jet through the iridotomy is produced. The resulting jet velocity and wall shear stress on the cornea are strongly dependent on the radius of the iridotomy and on the volume change of the posterior chamber. Our results suggest that there could be a risk of corneal endothelial cell detachment if the cornea is too close to the iridotomy and/or the volume change of the posterior chamber is sufficiently large.

Keywords
iridotomy, lubrication theory, regularised pressure

1.3.2 Sarangam Majumdar

Classical and numerical foundation theory: Parabolic evolution problems with application

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Abstract

This talk considers classical differential equations theory from the beginning of the mathematical analysis until present days perspective in general. We study in detail numerical foundation theory of the parabolic equations which arise in physics, chemistry, engineering and other branches of science. We begin our study with the formalism, the Gelfand triple, resolvent estimates. Then, the semigroup approach, which go back to the invention of the analytic semigroups in the middle of the last century, are characterized by precise formulas representing the solutions of the Cauchy problem for evolution equations.
Numerical foundation theory for parabolic evolution problems deal with time approximation. Explicit and implicit Euler scheme, Crank- Nicolson methods, explicit and implicit Runge-Kutta schemes are explored in a systematic manner. Stability property, smoothing property and convergence for all the schemes are presented. Then, we move on to Hilbertian integrals, the finite element semidiscretization, higher order methods, full discretization and the von Neumann criterian theory.

The second part of talk contain a complete new application of the parabolic evolution equation that appear in quorum sensing mechanism. We introduce a new mathematical model of quorum sensing system in bacteria. A convection - diffusion equation explain the complex biochemical density dependent phenomenon which is initiated around 1994 by a group of microbiologist. We explain the whole system and investigate stability with experimental data. Moreover, we apply different numerical schemes and compare the result with well mixed bacterial batch culture.

Finally, we study brusselator with numerical simulations. We apply different algorithm and compare them.

Keywords

finite element method, quorum sensing, brusselator

1.3.3 Marek Netušil[1], Willi Jäger[2], Jeremi Mizerski[3]

Multiscale modelling of the aortic media

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Abstract

Arterial wall is a complex three-dimensional structure composed of many constituents, e.g. elastin, collagen and smooth muscle cells. All these components have different mechanical and geometrical properties. Ability to appropriately model this structure is crucial for studies of the tissue growth and its mechanical behaviour (both healthy and pathological).
Purely phenomenological models are the most popular when it comes to the description of mechanical properties of blood vessel walls due to their "easy-to-understand" and "easy-to-implement" nature. However, their predictability and the ability to give answers about artery composition are very limited. Thus, the need for structure-based models arises.
Approach presented in the talk is based on the mathematical theory of homogenization. As the first step a detailed model of a mesoscopic structure is build. Then it is used to derive macroscopic properties of the tissue.

Keywords

blood vessel, aorta, multiscale modeling, homogenization

1.3.4 R. Malin Schemschat, Debora Clever, Katja Mombaur

Simulation based analysis of human push recovery motions using numerical optimization

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Abstract

As unperturbed motion barely exists in real world, it is extremely important for humans to be able to react on perturbation during their daily life tasks. In this work a dynamical two dimensional (2D) human model in sagittal plane is used to analyze perturbed human walking motions. Perturbation in form of pushes from the back at different height at the spine of varying strength during walking motions is regarded. Two kinds of optimal control problems are formulated: First, a least-squares objective function is used to fit the dynamical model to reference data gained from motion capture experiments. With this approach it is possible to analyze the resulting torques in the joints. Optimization allows to calculate physical quantities which cannot be measured. It is possible to include these quantities in the rating of different criteria that lead to a similar motion as the reference data. Therefore secondly, objective functions consisting of linear combinations of different criteria (as minimal end time, minimal energy, maximal step length, . . .) are formulated to generate motions of the human model from a given start posture. To solve the infinite dimensional optimal control problem, a direct multiple shooting approach is used. It is coupled with an efficient sequential quadratic programming (SQP) method to solve the resulting nonlinear program (NLP). The field of application of the results is broad: In sport sciences or medicine the better understanding of human motion can be used to improve training or therapies for athletes, injured, or elderly people. Control strategies and the even the design of prostheses, exoskeletons or humanoid robots for disabled people can be improved.

Keywords

multi-body simulation, human walking,push recovery, optimal control

1.4 Session THU-3.1 (Thu, 14:00 – 15:15, lecture hall H1)

1.4.1 Puya Latafat

Operator splitting techniques and their application to embedded optimization problems

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Abstract

Operator splitting techniques are algorithms that work by splitting a problem into smaller subproblems that are easier to solve. They can be used to solve problems arising in PDEs, monotone inclusions, variational inequalities and optimization. These methods were introduced in the 50's and have recently gained popularity due to their simplicity and applicability to large scale optimization problems such as the ones encountered in machine learning, signal processing and control. In the first part of this talk the classic splitting methods, Forward-Backward splitting(FBS) and Douglas-Rachford splitting(DRS) are discussed through simple examples.

Recent advances in primal-dual algorithms and their application to distributed optimization are considered in the second part of the talk. Many problems of interest involve large-scale, networked systems that are typically made up of many dynamical subsystems, or agents, that interact locally. Examples include power systems, sensor networks, formation control, water networks, etc. In most of these applications, there are computational or physical limits on the system that makes centralized approaches infeasible. The problems that we consider involve a network of agents interacting based on a communication graph. Each agent has its own private cost function. The goal is to minimize the aggregate of private cost functions and reach a consensus globally by only allowing limited exchange of information between neighbors. In particular, we consider a general scenario where the private cost function of each agent consists of the sum of three convex functions, one smooth with Lipschitzian gradient, and two possibly nonsmooth, one of which is composed with a linear operator. As an application we consider the Distributed Model Predictive Control (DMPC) problem. In the setting

of DMPC for each agent the smooth term can encode the local finite-horizon cost, and the other two nonsmooth functions can encode the linear dynamics with neighbors, and input and state constraints.

Keywords
convex optimization, monotone inclusion, operator splitting

1.4.2 Lia Strenge

It's all about power: definition, modeling and control of swarm type direct current microgrids

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Abstract

Energy from renewable sources is on the rise, in particular in Bangladesh. Stand-alone solar home systems are widely used to electrify rural areas without connection to the utility grid [1]. We study the interconnection of existing solar home systems in order to form an organically growing microgrid from the bottom up: the concept of swarm electrification. Households are enabled to trade energy between their former stand-alone systems. Hence, the energy service provision is improved with the existing installed capacity. Each solar home system is an energy producer and an energy consumer towards the grid, i.e. a prosumer, dependent on the energy needs of the household. The power flow control and the network topology optimization are of high interest for the design and operation of such grids [2].

We define the basic concepts of a solar home system, swarm electrification and a swarm type low voltage direct current (DC) microgrid. We present an overview on possible modeling and simulation frameworks and define the corresponding interfaces to applied mathematics for further understanding of the underlying theory. Exemplarily, we derive a physical model of a swarm type low voltage DC microgrid as a basis for future control design in accordance with the research and development in practice. The present model is a nonlinear differential-algebraic equation system of arbitrarily high dimension depending on the number of interconnected households and the network topology. In addition, the switching between consumer and producer of a solar home system is reflected. For control purpose, we define different control objectives regarding voltage stability and power sharing in the grid and show that droop control is a suitable first decentralized control approach. Further research is needed regarding optimized power flow control and stability analysis for arbitrary network topologies taking into account multi-objective cost functions and data analysis of the pilot project in practice.

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[2] A. Magnasco, H. Kirchhoff, S. Chowdhury and S. Groh. Data Services for Real Time Optimization of DC Nanogrids with Organic Growth. *Energy Procedia*, Elsevier, 2016.

Keywords

differential-algebraic equation, control, optimization, swarm type DC microgrid

1.4.3 Sven Leyffer[1], Anna Thünen[2]

Rounding based heuristics for mixed-integer partial differential equation constrained optimization

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Abstract

A new class of mixed-integer partial differential equation constrained optimization
(MIPDECO) has been established recently. It combines two key classes of optimization, namely mixed-integer nonlinear optimization (MINLP) and partial differential equation (PDE) constrained optimization. In MINLP the feasible set and the objective are quantified by nonlinear functions. In addition to continuous decision variables, we have to deal with integer variables leading to combinatorial difficulties. These difficulties arise from making decisions which are coded on an enumerable set of feasible options. On the other hand, many applications in optimization involve complex systems which might be modeled by partial differential equations. PDE constrained optimization poses different challenges since it leads to a large number of variables and numerical complexity, so both problem classes are studded with big challenges. As different as these subfields are, so different and less compatible are their solution approaches. Hence we need to develop new solution approaches to overcome the challenges both of integer variables and the number of variables. This is of importance since MIPDECO has a broad range of applications, in particular: topology optimization, design and control of gas networks, as well as in technology of both renewable and conventional energies.

Unfortunately, we can solve the studied problems only on very coarse meshes. To get a meaningful solution we would need to use finer meshes which then causes a significant increase in the number of variables and constraints. Therefore we present tailored rounding-based heuristics and results.

Keywords
MIPDECO, MINLP, PDE optimization

1.5 Session FRI-1 (Fri, 09:00 – 10:40, lecture hall H1)

1.5.1 Bastian Rieck

A primer in persistent homology

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Abstract

The field of computational topology started to gain a large amount of traction over the last few years. It provides novel data analysis methods that are firmly rooted in algebraic topology, differential topology, and linear algebra. In my talk, I aim to give an introduction to *persistent homology*, a method that has proven to be very effective in characterizing as well as summarizing complex behaviour in multivariate data. I will briefly explain the necessary mathematical basis for this novel technique and focus on building up the intuition behind it. Furthermore, I will use examples from scalar field analysis in order to demonstrate the capabilities of persistent homology.

Keywords

computational topology, persistent homology, multivariate data

1.5.2 Ole Klein

Parameter Estimation and Uncertainty Quantification for Flow and Transport Processes

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Abstract

The modeling of flow and transport processes in porous media poses several challenges, both conceptual and computational. Detailed knowledge about the state variables is typically limited to discrete spatial and temporal observation points, while the underlying parameters of the models are spatially heterogeneous and can vary over several orders of magnitude. This makes the identification of system parameters and reliable predictions based on model outcomes difficult. Matters are complicated by unavoidable measurement noise and the high cost of simulations.

We present a method for Bayesian inversion based on preconditioning and the use of randomized algorithms. This approach provides a linearization of the posterior distribution of the parameters conditioned on the measurements, incorporating both uncertainty of the parameters and measurement noise. Preconditioning and randomization lead to mesh-independent convergence rates and a cost that is largely decoupled from the number of observations, making this method especially suitable for high-resolution parameter estimation based on large data sets. The approach provides statistical consistency checks at no additional cost, which can be used to check the validity of the linearized distribution.

Keywords

parameter estimation, uncertainty quantification, large data sets

1.5.3 Sven de Vries, Jan Pablo Burgard, Ulf Friedrich, Dennis Kreber

A Minimum-Cost Flow Approach for Solving Statistical Imputation Problems

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Abstract

Almost all population surveys suffer from missing responses, inhibiting the direct application of estimation methods requiring full data sets. To create one complete and coherent data set, usually single imputation method are applied. A prominent single imputation variant is the nearest neighbor hot deck imputation. It replaces the missing values with observed values from the closest donor with respect to a distance, e.g. the Gower distance. To avoid a repeated assignment of donors to non-respondents and thus a distortion of the distribution, the proposed method limits the number of maximum donations per unit. This setup leads to a simple, weighted *b*-matching problem, which can be transformed to a minimum-cost flow problem.

The proposed method is compared to existing single imputation methods within a large scale Monte-Carlo simulation based on the Amelia dataset. The estimation of a total is studied under different missing patterns for a variety of variables, e.g. the income. Variance estimation is performed via bootstrap. The Monte-Carlo simulation indicates that the imposed restriction on the reuse of donors may lead to a lower bias and variance.

Keywords

single imputation, hot deck imputation, nearest neighbor, b-matching, minimum-cost flow

1.5.4 Martin Rupp, Ralf Muennich

Numerical optimization for multivariate optimal allocation problems with several levels of strata

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Abstract

In Survey Statistics, the aim of modern surveys is to draw a sample which provides accurate information on a large variety of characteristics as well as on different regional levels and other subclasses of a population. Hence, optimal allocation of a fixed sample size to the strata has to consider a vast number of strata along with optimization conflicts due to the complementary information of the characteristics of interest. Furthermore, particular quality or cost restrictions might be taken into account.

Modelling this multivariate optimal allocation problem leads to a multi-objective optimization problem with equality constraints and box-constraints. Taking advantage of the special structure of the objective functions and applying Pareto-optimization, the problem can be equivalently reformulated as a significantly lower dimensional non-linear system of equations, depending only on the Lagrange multipliers.

Even though this system is non-smooth, it can be solved applying a semi-smooth newton algorithm with appropriate starting point and step size strategies. Due to the lower dimension, computational time is reduced considerably. The performance of the developed algorithm is tested on a business data set.

Keywords
Survey Statistics, optimal allocation, Pareto-optimization, semi-smoothness, box-constraints

1.6 Session FRI-2 (Fri, 11:00 – 12:40, lecture hall H1)

1.6.1 Alessandro Arrigoni, Klaus Engel[1]

A semigroup approach to boundary feedback systems

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Abstract

In this talk we convert a class of boundary feedback systems with delay into an Abstract Cauchy Problem; by means of recent results on semigroup theory, we study well-posedness and stability of the original systems.

Keywords

boundary feedback with delay, C_0-semigroups, operator matrices

1.6.2 Björn Baran, Peter Benner, Jan Heiland

Optimal Control of a Stefan Problem System Fully Coupled with Navier-Stokes Equations and Mesh Movement

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Abstract

Free boundary and moving boundary problems, that can be used to model crystal growth or the solidification and melting of pure materials, receive growing attention in science and technology. The optimal control of these problems appear even more interesting since certain desired shapes of the boundaries improve, e.g., the material quality in the case of crystal growth.

We consider the so called two-phase Stefan problem that models a solid and a liquid phase separated by a moving interface ($\Gamma_{\text{interface}}$). In both phases the heat distribution T is characterized by the heat equation. The fluid flow in the liquid phase is described by Navier-Stokes equations. The interface movement is coupled with the temperature through the Stefan condition (1.1). This condition connects the normal velocity of the interface $V_{\text{interface}}$ to the jump of the temperature gradient across the interface:

$$[k_s(\nabla T)_s - k_l(\nabla T)_l] = L \cdot V_{\text{interface}}, \qquad \text{on } \Gamma_{\text{interface}}. \tag{1.1}$$

In the work presented, we take a sharp interface model approach and define a quadratic tracking-type cost functional that penalizes the deviation of the interface from the desired state at a final time as well as the control costs. Following the "optimize-then-discretize" paradigm, we formulate a first order optimality system using the formal Lagrange approach and derive the adjoint PDE system that provides the needed gradient of the cost functional.

By means of an example setup of a container with in- and outflow boundaries, we illustrate how the derived formulations can be used to achieve a desired interface between the solid and the fluid phase by controlling the flow at the inlet. Among other implementation issues, we address how to handle the weak discontinuity of the temperature along the interface in a finite element framework with mesh movement methods.

Keywords
optimal control, adaptive method, moving finite elements, moving boundary, phase change, Stefan problem

1.6.3 Francesco Ludovici

Optimal Control of Parabolic PDEs with State Constraints
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Abstract

Optimal control problems governed by parabolic partial differential equations (PDEs) and subject to limitations on the state variable arises in many fields of applied science and industry. Steel production, crystal-growth and stress control are some of the possible applications.

For a thoroughly treatment of this class of problem a time-space discretization is required. As a consequence, we derive convergence rates for the state and control variables as temporal and spatial mesh sizes tend to zero. We will show the tools and mathematical challenges behind the derivation of such convergence rates, for the case of a linear and nonlinear PDE.

Keywords
finite elements, state constraints, convergence

1.6.4 Manuela Hund, Jens Saak

A Connection between Time Domain Model Order Reduction and Moment Matching

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Abstract

The open literature provides a variety of projection based model order reduction (MOR) methods for linear input-output systems as

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t), \end{aligned} \tag{1.1}$$

with a regular matrix $E \in \mathbb{R}^{n\times n}$, as well as matrices $A \in \mathbb{R}^{n\times n}, B \in \mathbb{R}^{n\times p}$ and $C \in \mathbb{R}^{q\times n}$.

Jiang and Chen introduced a unifying framework for time domain MOR based on general families of orthogonal polynomials. Their method leads to a large linear system of equations

$$Hv = f. \tag{1.2}$$

The solution vector v is used to compute the projection matrix for dimension reduction. Searching for a reduced order model of order m, (1.2) has dimension $m \cdot n$. Hence, (1.2) easily becomes too large to solve even on recent computers.

Since (1.2) is well structured, and also sparse if E and A are sparse matrices, Jiang and Chen propose an iterative Jacobi-like solution method exploiting this structure. However, it is known that this method often converges slowly. In addition, we can show that the matrix H in (1.2) is not regular in general.

Exploiting the structure of H we show a connection to a Sylvester equation

$$AVO + EVP = F, \tag{1.3}$$

where A and E denote the coefficient matrices in (1.1). O and P are structured, small and depend only on the choice of the family of orthogonal polynomials. The right-hand side f and solution vector v of (1.2) can be obtained by reshaping F and V stacking their columns on top of each other.

Our approach computes the matrix V by solving a (regularized) Syl-

vester equation (1.3) rather than the linear system (1.2).

Under mild conditions (see, e.g. Vandendorpe's PhD thesis) this Sylvester equation is directly connected to a rational Krylov subspace and hence to interpolatory MOR and moment matching. Depending on the choice of orthogonal polynomials we show that these conditions are always fulfilled.

In that case time domain model order recduction based on orthogonal polynomials is an interpolation method with expansion points only depending on the choice of orthogonal polynomials, not on characteristics of the system to reduce. Hence, this MOR method is necessarily inferior to other reduction methods choosing their expansion points according to the system (e.g, the iterative rational Krylov algorithm (IRKA)).

Keywords

time domain model order reduction, orthogonal polynomials, moment matching

2 Posters

1. **On numerical study of Parkinson tremor**
   - **Author**: Annalakshmi Harikrishna
     (with Dennis Effah Osei, Magdalena Weronika Kamińska, Sarangam Majumdar)
   - **Institution**: Universit*à* degli Studi dell'Aquila (Italy)
   - **Description**: Parkinson's disease and Parkinson's tremor are the two most common movement disorders, nor do we fully understand the origin of one of the disease's cardinal symptom: the Parkinsonian tremor. We study one mathematical model involved in Parkinson's disease and in the Parkinsonian tremor, use the Van der Pol equation to further understand this tremor as well as investigate different numerical approaches to solve the system and compare them.
   - **Keywords**: Parkinson tremor, Van der Pol equation, Oscillation

2. **Application of the cut-off projection on the 1D backward heat conduction problem in a two-slab system**

    - **Author**: Tran The Hung
    (with Vo Anh Khoa, Gran Sasso Science Institute (Italy), and Mai Thanh Nhat Truong, Hankyong National University (Republic of Korea))
    - **Institution**: University of Hamburg (Germany)
    - **Description**: Instability in ill-posed problems is one of the most interesting field in PDE models. Many approachs have been conceived in order to stabilize the solution. The main concern of this work is the cut-off projection for the one-dimensional backward heat conduction problem in a two-slab system with perfect contact. In a constructive manner, we commence by demonstrating the Fourier-based solution that contains the exponential growth due to the natural high frequency of Fourier series which leads to instability. In other words, such instability motivates our detailed study of projection where the cut-off approach is derived consistently. In theoretical framework, the first two achievements are to construct the regularized problem and devise its stability for each noise level. Our second interest would be the error estimates over the L^2-norm as the exact solution belongs to H^1. Interestingly, the logarithmic-type convergence rate is obtained as well. All in all, this work can be considered as a preliminary attempt for the two-slab system backward in time. A simple numerical test is provided to corroborate the qualitative analysis. Finally, the conclusions and discussions about another promising results are given at the end of this presentation.
    - **Keywords**: backward heat equation, two-slab system, cut-off projection, ill-posedness, stability, error estimate, computing

3. **Examples of evolutionary Γ-convergence**
    - **Author**: Thomas Frenzel
      (with Alexander Mielke)
    - **Institution**: WIAS Berlin
    - **Description**: The objects of investigation are parameter-dependent parabolic semi-linear PDEs which are gradient flows induced by an energy functional $\mathcal{E}_\varepsilon$ and a dissipation potential $\mathcal{R}_\varepsilon$. Different models are presented where the framework of evolutionary Γ-convergence is applicable. All problems inherit different time or spatial scales.

      One special class are wiggly energy models. Here the number of solutions to the stationary equation $0 = -\mathrm{D}\mathcal{E}_\varepsilon$ tends to infinity as $\varepsilon \searrow 0$ but the evolution is still unique and the limiting process leads to a change in the structure of the dissipation potential.

      Another class are highly non-convex problems where the limit equation can be described as a perturbed gradient flow which might be not uniquely solvable.
    - **Keywords**: parabolic semi-linear PDE, gradient flow, evolutionary Γ-convergence, multiscale, wiggly energy models, delamination

4. **Breathing modes of parametric driven sine-Gordon equation with phase shift**

    - **Author**: Taj Munir
    (with Amir Ali, University of Malkand Dir Lower (Pakistan), Hussan Zeb, Hazara University (Pakistan))
    - **Institution**: University of Magdeburg (Germany)
    - **Description**: We consider a non-homogeneous parametric driven sine-Gordon equation with phase-shift describing a long Josephson Junction, driven by a micro wave field. We construct a perturbative expansion for breathing mode to obtain equations for slow time evolution of oscillation amplitude. Multiple scale expansions are used to determine whether the external drive can excite the defect mode of a junction. Large oscillation amplitude along with high frequency drive is provided to the system for rapid oscillation. Along side, energy input given by the external drive versus energy out put due to radiative damping experience produces energy balance leading to small drive amplitude. We expected that the modes decay algebraically in time due to the energy transfer from the discrete to the continuous spectrum.
    - **Keywords**: breathing modes, josephson junction, mutiple scale expansion

5. **Modelling of reactive multiphase flow and heat transfer in fluidized bed reactor**
   - **Author**: Vít Orava
     (with Ondřej Souček, Charles University in Prague (Czech Republic), and Peter Čendula, Zürich University of Applied Sciences (Switzerland))
   - **Institution**: Charles University in Prague (Czech Republic)
   - **Description**: We investigate a prototype concept of a back-up electricity device where we use liquid formic acid (*FA*) to produce a mixture of carbon dioxide (CO_2) and hydrogen (H_2) which is used in a PEM fuel cell. Gaseous H_2 is produced by endothermal decarboxylation of *FA* performed by heterogeneous solid-based catalysis in fluidized bed multi-phase reactor. The modeling of this reactor is the main focus of this work. The outcoming gaseous mixture flows into a PEM fuel cell.

     In the fluidized bed reactor the liquid formic acid is decomposed to a gaseous mixture of CO_2 and H_2 in the presence of microscopic floating solid catalytic particles. We describe the system, contained in a fixed control volume, as a mixture composed of four constituents – formic acid, catalyst microparticles (*Cat*), carbon dioxide and hydrogen. For the individual mixture components, we distinguish partial densities and momenta, while we only consider one common temperature field for the mixture as a whole. We reduce the four-constituents model to a binary mixture model of liquid phase ($Cat + FA$) and gaseous phase ($CO_2 + H_2$) which forms bubbles. The liquid phase is considered as a compressible viscous fluid with temperature-dependent density and viscosity depending on both the temperature (Arrhenius model) and the volume fraction of the catalyst particles. Physical interaction between the bubbles and the liquid is modeled under simplifying assumptions by the pressure-drag balance. The chemical rates satisfy mass-action law and follow the Arrhenius kinetics.

     The model was implemented numerically in COMSOL Multiphysics and we present several simulations addressing primarily the role of liquid viscosity and imposed wall temperature on the performance and flow regime inside the reactor.

- **Keywords**: fluidized bed reactor, multiphase flow, model reduction, bubbly flow, Arrhenius kinetics

6. **Development of algorithmic strategies for numerical simulation of coupled mechanical-diffusion problems**
    - **Author**: Jorge De Anda Salazar
      (with Laurent Stainier, Thomas Heuzé)
    - **Institution**: Ecole Centrale de Nantes (France)
    - **Description**: The aim of the research is the exploration of novel algorithms strategies for numerical simulation of non-linear strongly coupled mechanics-diffusion problems. The former is based on a proposed variational formulation approach which provides a natural framework for coupled problems, with numerical benefits such as efficiency, flexibility and robustness in algorithms overcoming classical results. Through a variational formulation, the solution for a mechanics-diffusion problem can be stated as an optimization process.

      A description for the development and numerical implementation of a variational formulation for transient-diffusion boundary-value problem will be presented. In specific, a non-linear model and its linearized version are solved for a "concentration-shock" problem. The numerical results obtained are compared against classical methods derived from a weak formulation. The spatial discretization is done using a finite element approach in all cases. Temporally, the Crank-Nicolson and an Implicit discretization are used for the weak derived schemes, while for the variational formulation an implicit-explicit is selected.

      The goal of the variational formulation for transient diffusion problems is in our interest since it settles a path to follow for the modeling and resolution of coupled problems. Mechanical-diffusion problems, provide a wide range of applications among many fields, from reactive flows in solids to tissue reconstruction by means of hydrogels, among others.
    - **Keywords**: variational formulation, coupled problems, discrete variational formulation, irreversible processes

7. **Optimal Control Problems in Thermoviscoplasticity**
    - **Author**: Ailyn Stötzner
      (with Roland Herzog, Technische Universität Chemnitz (Germany), and Christian Meyer, Technische Universität Dortmund (Germany))
    - **Institution**: Technische Universität Chemnitz (Germany)
    - **Description**: Elastoplastic deformations play a tremendous role in industrial forming. Many of these processes happen at non-isothermal conditions. Therefore, the optimization of such problems is of interest not only mathematically but also for applications.

      On our poster we will present the analysis of the existence of a global solution of an optimal control problem governed by a thermovisco(elasto)plastic model. We will point out the difficulties arising from the nonlinear coupling of the heat equation with the mechanical part of the model. Finally, we can discuss first steps to develop an efficient optimization method based on the directional differentiability of the control-to-state mapping.
    - **Keywords**: thermoviscoplasticity, variational inequality of second kind, maximal parabolic regularity, optimal control

8. **Numerical Approximation of the eXtended Fluid-Structure Interaction (eXFSI) Problem**
    - **Author**: Bhuiyan Shameem Mahmood Ebna Hai (with Markus Bause)
    - **Institution**: Department of Mechanical Engineering, The Federal Armed Forces University Hamburg (Germany)
    - **Description**: This contribution is the part of the research work on Finite Element Model-based Structural Health Monitoring (SHM) Systems, where we introduce a monolithic variational formulation and solution techniques of eXtended Fluid-Structure Interaction (eXFSI) Problem. To the best of our knowledge, such a model is new in the literature. This model is used to design an on-line structural health monitoring (SHM) system in order to determine the coupled acoustic and elastic wave propagation in moving domains and optimum locations for SHM sensors. In a monolithic nonlinear fluid-structure interaction (FSI), the fluid and structure models are formulated in different coordinate systems. This makes the FSI setup of a common variational description difficult and challenging. This article presents the state-of-the-art in the finite element approximation of FSI problem based on monolithic variational formulation in the well-established arbitrary Lagrangian Eulerian (ALE) framework. This research focuses on the newly developed mathematical model of a new FSI problem, which is referred to as extended Fluid-Structure Interaction (eXFSI) problem in the ALE framework. The eXFSI is a strongly coupled problem of typical FSI with a coupled wave propagation problem on the fluid-solid interface (WpFSI). The WpFSI is a strongly coupled problem of acoustic and elastic wave equations, where wave propagation problems automatically adopts the boundary conditions from the FSI problem at each time step. The ALE approach provides a simple but powerful procedure to couple solid deformations with fluid flows by a monolithic solution algorithm. In such a setting, the fluid problems are transformed to a fixed reference configuration by the ALE mapping. The goal of this work is the development of concepts for the efficient numerical solution of eXFSI problem, the analysis of various fluid-solid mesh motion techniques and comparison of different second-order

time-stepping schemes. This work consists of the investigation of different time stepping scheme formulations for a nonlinear FSI problem coupling the acoustic/elastic wave propagation on the fluid-structure interface. Temporal discretization is based on finite differences and is formulated as a one step-θ scheme, from which we can consider the following particular cases: the implicit Euler, Crank-Nicolson, shifted Crank-Nicolson and the Fractional-Step-θ schemes. The nonlinear problem is solved with a Newton-like method where the discretization is done with a Galerkin finite element scheme. The implementation is accomplished via the software library package DOpElib based on the `deal.II` finite element library for the computation of different eXFSI configurations.

- **Keywords**: fluid-structure interaction, finite element method, finite elements based SHM, interaction between wave/field and structure/material, guided waves, elastic wave propagation