14th International Conference
June 5 - 9, 2023
Sozopol, Bulgaria

LARGE-SCALE SCIENTIFIC COMPUTATIONS

LSSC'23

Scientific Program
Abstracts
List of Participants

Institute of Information and Communication Technologies
Bulgarian Academy of Sciences

PREFACE

The fourteenth International Conference on "Large-Scale Scientific Computations" LSSC 2023 is organized by the Institute of Information and Communication Technologies, Bulgarian Academy of Sciences.

A wide range of recent achievements in the field of scalable numerical methods, algorithms and their applications will be addressed during the conference. The meeting provides a forum for exchange of ideas between scientists, who develop and study numerical methods and algorithms, and researchers, who apply them for solving real life problems.

The major scientific topics include: Hierarchical, adaptive, domain decomposition and local refinement methods; Robust preconditioning algorithms; Monte Carlo methods and algorithms; Numerical linear algebra; Control systems; Parallel algorithms and performance analysis. Large-scale computations of environmental, biomedical and engineering problems.

LIST OF PLENARY INVITED SPEAKERS:

Boian Alexandrov (Los Alamos National Laboratory, USA)
Daniele Boffi (King Abdullah University of Science and Technology, Saudi Arabia)
Maya Neytcheva (Uppsala University, Sweden)
Géraldine Pichot (INRIA, Paris, France)
Joachim Schöberl (Vienna University of Technology, Austria)
Ivan Yotov (University of Pittsburgh, USA)

LIST OF SPECIAL SESSIONS:

- Preconditioning and Multilevel Methods, In memory of Owe Axelsson
  organized by Maya Neytcheva (Uppsala University, SE), Panayot Vassilevski (Portland State University, US)

- Fractures and Mixed Dimensional Modeling: Discretizations, Solvers, and Methodology
  organized by James Adler, Xiaozhe Hu (Tufts University, US), Géraldine Pichot (Inria, FR), Ludmil Zikatanov (Penn State University, US)

- Modeling, Discretization and Solvers for Interface-Coupled Multiphysics Problems
  organized by Ana Budisa, Miroslav Kuchta, Kent-Andre Mardal (University of Oslo, NO), Ludmil Zikatanov (Penn State University, US)

- Machine Learning and Model Order Reduction for Large Scale Predictive Simulations
  organized by Bernard Haasdonk (University of Stuttgart, DE), Oleg Iliev (ITWM, Kaiserslautern, DE), Mario Ohlberger (University of Münster, DE)

- Fractional Differential Problems: Theoretical Aspects, Algorithms and Applications
  organized by Lidia Aceto (University of Eastern Piedmont, Alessandria, IT), Stanislav Harizanov (IICT-BAS, BG)

- Variational Analysis and Optimal Control
  organized by Mikhail Krastanov (Sofia University, BG), Vladimir Veliov (TU Wien, AT)

- Stochastic Optimal Control and Numerical Methods in Economics and Finance
  organized by Daria Ghilli (University of Pavia, IT), Marta Leocata (LUISS Guido Carli, IT), Giulia Livieri (School Normal Superior, IT)

- Tensor Methods for Big Data Analytics and Low-Rank Approximations of PDEs Solutions
  organized by Boian Alexandrov (Los Alamos National Laboratory, US), Hristo Djidjev (IICT-BAS, BG), Gianmarco Manzini (Los Alamos National Laboratory, US)

- Applications of Metaheuristics to Large-Scale Problems
  organized by Stefka Fidanova (IICT-BAS, BG), Gabriel Luque (University of Malaga, ES)

- Large-Scale Models: Numerical Methods, Parallel Computations and Applications
  organized by Krassimir Georgiev (IICT-BAS, BG), Zahari Zlatev (Aarhus University, DK)

- HPC and Big Data: Algorithms and Applications
  organized by Aneta Karaivanova (IICT-BAS, BG), Todor Gurov (IICT-BAS, BG), Emanouil Atanassov (IICT-BAS, BG)

This booklet contains the scientific program (Part A), abstracts of the conference talks (Part B), the list of participants (Part C).

Acknowledgement
The conference is organized with the financial support of the Bulgarian National Science Fund under Contract KP-06-MNF-35/16.12.2022. The Bulgarian National Science Fund is not responsible for the content of the talks presented at the scientific forum, as well as for the content of advertising materials and other materials for it.

The organizers

June 2023

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[1] All times are EEST (GMT+3).

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09:55 - 10:20	V. Ivanov, G. Gadzhev, I. Georgieva, K. Ganev, N. Miloshev, Influence of the Grid Resolutions on the Computer Simulated Air Quality Indices Over the Territory of Bulgaria
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Part B

Abstracts[2]

[2]Arranged alphabetically according to the family name of the first author.

The Generalized Residual Cutting Method and its Convergence Characteristics

T. Abe, A. T. Chronopoulos

Iterative methods and especially Krylov subspace methods (KSM) are a very useful numerical tool in solving for large and sparse linear systems problems arising in science and engineering modeling. More recently, the nested loop KSM have been proposed that improve the convergence of the traditional KSM. In this work, we review the residual cutting (RC) and the generalized residual cutting (GRC) that are nested loop methods for large and sparse linear systems problems. We show that GRC, in exact arithmetic, is equivalent to Orthomin with a variable polynomial preconditioning. We use the modified Gram-Schmidt method to derive a stable GRC algorithm. We show that GRC presents a general framework for constructing a class of "hybrid" (nested) KSM based on inner loop method selection. We conduct numerical experiments using nonsymmetric indefinite matrices from a widely used library of sparse matrices that validate the efficiency and the robustness of the proposed methods.

Efficient Computation of the Wright Function and Its Applications to Fractional Diffusion-Wave Equations

L. Aceto, F. Durastante

In this talk, I'm going to present a new algorithm for the efficient computation of the Wright function:

$$W_{\lambda,\mu}(z) := \sum_{n=0}^{\infty} \frac{z^n}{n!\,\Gamma(\lambda n + \mu)}, \quad \lambda > -1,\ \mu \in C.$$

I'll focus on the cases of interest for the expression of solutions of some fractional differential equations. The proposed algorithm is based on the inversion of the Laplace transform of a particular expression of the Wright function:

$$f_{\lambda,\mu}(t;x) := t^{\mu-1} W_{\lambda,\mu}(-|x|t^{\lambda}), \qquad t \geq 0,\ x \in R, \quad \lambda \in (-1,0),\ \mu \in C.$$

The Laplace transform inversion corresponds to the computation of the Bromwich integral

$$f_{\lambda,\mu}(t;x) = \frac{1}{2\pi i} \int_{\mathcal{C}} e^{st} F_{\lambda,\mu}(s;x)\,\mathrm{d}s, \qquad F_{\lambda,\mu}(s;x) = s^{-\mu} e^{-|x|s^{-\lambda}}.$$

To determine the number of quadrature nodes and a suitable transform of the Bromwich line $\mathcal{C}$, we utilize the error analysis for obtaining a result with a certified bound. The proposed procedure is innovative with respect to previous attempts in the literature because it avoids dealing with oscillatory integrals and is fairly easy to implement.

The algorithm is also made available in the form of a code package implementing the inversion procedure proposed here in different programming languages (Fortran 2018, Matlab) for *single*, *double*, and *quadruple* precision.
I'll illustrate the analysis with a set of numerical experiments validating both the theoretical estimates of the error and the applicability of the proposed method for representing the solutions of fractional differential equations on unbounded domains.

A Rational Preconditioner for Multi-dimensional Riesz Fractional Reaction-diffusion Equations

L. Aceto, M. Mazza

In this talk we propose a rational preconditioner for an efficient numerical solution of linear systems arising from the discretization of multi-dimensional Riesz fractional reaction-diffusion equations. In particular, the discrete problem is obtained by employing finite difference or finite element methods to approximate the fractional derivatives of order α with $\alpha \in (1, 2]$. The proposed preconditioner is then defined as a rational approximation of the Riesz operator expressed as the integral of the standard heat diffusion semigroup. We show that, being the sum of k inverses of shifted Laplacian matrices, the resulting preconditioner belongs to the generalized locally Toeplitz class, a wide algebra of matrix sequences that can be linked to a function representing the asymptotic eigenvalue distribution as the matrix size diverges. As a consequence, we are able to provide the asymptotic description of the spectrum of the preconditioned matrices and we show that, despite the lack of clustering just as for the Laplacian, our preconditioner for α close to 1 and $k \neq 1$ reasonably small, provides better results than the Laplacian itself, while sharing the same computational complexity.

SmartTensors: A New AI Platform for Big-Data Analytics and Feature Extractions

B. Alexandrov

Large amounts of high-dimensional data are constantly being generated all over the globe by massive computer simulations, sensors and sensor networks, electronic surveillance, mobile devices, etc. Utilizing such big-data for decision making, emergency response, and data-driven science requires clear understanding of the processes underpinning the data. In big-data analytics, it is difficult to directly link the data to the underlying processes, since the datasets are formed exclusively by observable quantities, while the original processes/features remain mixed and latent (not directly observable). Extracting these latent features can not only reveal valuable information about previously unknown causalities and mechanisms hidden in the data, but also uncovers low-dimensional latent structure by which the entire dataset is represented and interpreted. Here, we present our

groundbreaking unsupervised software tool, **SmartTensors** AI, based on Non-negative Tensor Factorization and Tensor Networks. **SmartTensors** is an unsupervised AI platform capable of extracting easy explainable latent features and performing analysis of large dynamic networks. The uniqueness of **SmartTensors** is that it estimates the latent dimension of large and diverse datasets, e.g., of size up to ˜350TB dense, and ˜10EB sparse datasets, and can analyze their structure and hidden physical processes.

On Some Quadratic Eigenvalue Problems

A. B. Andreev, M. R. Racheva

In a number of second- and fourth-order boundary value problems the spectral parameter λ appears quadratically as well as linearly. The paper deals with eigenvalue problems of this type. Here, an approach for linearization is proposed for both second- and fourth-order problems. By suitable substitution, a variational system is obtained in which spectral parameter λ appears only linearly but not quadratically.
Theoretical and computational aspects are considered. Combining linearization and the mixed method for fourth-order problems is also discussed. Finally, numerical results are presented.

Vaccination and Waning Immunity Model for Covid-19

G. Angelov, R. Kovacevic, N. I. Stilianakis, V. M. Veliov

Waning immunity models used in epidemiology can provide insights for the implementation of vaccination strategies and can help public health decision making. An optimal control epidemiological model is presented that is suitable for describing the evolution of Covid-19 and other diseases. Increase in immunity protection is provided either by infection or from vaccination, but the protection level wanes over time due to the diminishing antibodies and other factors. The protection level of an individual influences not only his susceptibility and recovery, but also his infectiousness and mortality chance. The model uses a system of first order PDEs that represents the evolution of a disease within the compartments of susceptible, infected, and vaccinated individuals, regarding the heterogeneity with respect to the immunity level. An optimal control problem is considered, with an objective functional depending on the number of infected individuals and the cost of vaccination. Numerical simulations with various parameters are used for quantitative comparison between optimal vaccination strategies.

Discontinuos Galerkin Approximation of the Fully-Coupled Thermo-Poroelastic Problem

P. F. Antonietti, S. Bonetti, M. Botti, I. Mazzieri

Poroelasticity inspects the interaction among fluid flow and elastic deformations within a porous medium. In several applications in the context of environmental sustainability, such as geothermal energy production and CO2 sequestration, temperature plays a key role in the description of the physical phenomena. Moreover, the thermo-poroelastic model finds application in the context of seismicity and induced seismicity.
In order to correctly describe these processes, the differential problem should also take into account the influence of the temperature, leading to a fully-coupled thermo-poroelastic (TPE) system of equations. In the framework of geosciences applications, the subsoil is modelled as a fully-saturated poroelastic material under the additional assumptions of small deformations and quasi-static regime. We present and analyze a discontinuous Galerkin method for the numerical modelling of the non-linear fully-coupled thermo-poroelastic problem. For the spatial discretization, we design a high-order discontinuous Galerkin method on polygonal and polyhedral grids (PolyDG) based on a novel four-field formulation of the problem. To handle the non-linear convective transport term in the energy conservation equation we adopt a fixed-point linearization strategy and different linearizations are examined. We perform a robust stability analysis for the linearized semi-discrete problem under mild requirements on the problem data. A priori hp-version error estimates in suitable energy norms are also derived. A complete set of numerical simulations is presented in order to validate the theoretical analysis, to inspect numerically the robustness properties, and to test the capability of the proposed method in a practical scenario inspired by a geothermal problem.proposed method in a practical scenario inspired by a geothermal problem.
To correctly describe the seismic case, the study of the fully-dynamic TPE problem is necessary. For this reason, recent advances in PolyDG discretization of wave propagation in thermo-poroelastic media will also be presented.

The Clarke Tangent Cone to the Epigraph of an Integral Functional

S. Apostolov, M. Krastanov, N. Ribarska

We consider a continuous integrand $L : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}$ and the integral functional φ stemming from L as a functional defined on $L^\infty([a,b],\mathbb{R}^n) \times L^1([a,b],\mathbb{R}^n)$. We are interested in the Clarke tangent cone to the epigraph of φ at a reference point $(\bar{x},\bar{y})$. Under suitable assumptions on L akin in nature to the ones used in [1], we show that the prepolar of the Clarke tangent cone to the epigraph of φ at the reference point consists of selections of normals to the epigraph of L at the point $(\bar{x}(t),\bar{y}(t))$ as t runs through $[a,b]$.

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Coefficient Restoration in a Fractional Honeybee Population Dynamics and Food Interaction Model

A. Atanasov, S. G. Georgiev, L. G. Vulkov

The overall honeybee colony number is steadily decreasing in the last decades. It is found that there are many causes for this dangerous phenomenon, and it is not a single reason but a combination of factors that causes such a decline. A powerful tool to study natural processes is the mathematical modelling. To support such a study, compartment differential models of honeybee population dynamics are typically involved.
In our investigation, we adopt a model comprising the main classes of bees, these are the brood, the young hive bees and the mature forager bees as well as the food stores of the colony. The food availability in the nature and the ability of the bees to collect it, reflected in the food storage in the hive, are proved to greatly influence the colony development. On the other hand, the memory effect of the dynamical system is activated by the usage of fractional-order derivatives in the model.
However, the true values of some of the most important parameters in the model are usually unknown and not directly measurable. In the paper, a coefficient identification inverse problem is solved via minimization of a quadratic error functional. Computational experiments with quasi-real data are performed to verify the properties of the proposed algorithm.

Solving the Montain Car Problem Using Genetic Algorithms

A. Bădică, C. Bădică, I. Buligiu, L. I. Ciora, M. Ganzha, M. Paprzycki

The Mountain Car problem (MCP) is a standard benchmark for experimenting with reinforcement learning and optimal control algorithms. MCP assumes an autonomous car driving on a one-dimensional track that follows a mountain range with the goal of reaching the mountain top in a minimum number of steps.
The aim of this paper is to investigate the suitability of using Genetic Algorithms (GA) for solving this problem. Actually we consider that MCP is a challenge for GA for the reason that the evaluation of the fitting function of a possible solution is rather costly, involving a complete simulation of the car movement to determine the effectiveness of a given policy for solving the MCP.
We briefly introduce the model of the MCP and the general outline of GA. We consider a discrete model of the problem, following our own approach introduced in a previous paper. We then present our solution by mapping the standard components of GA to our concrete problem. A solution corresponds to a policy that defines the car actions in each system state. The fitting function represents the time required by the car to reach the goal. This value is determined as the number of steps required to reach the goal. The GA manages a population of possible

solutions by applying genetic operators with the aim to minimize the fitting of solutions. The evaluation of the fitting function assumes the numerical simulation of the car movement under a given policy representing a possible solution. A policy can be pure or mixed. In a mixed policy, the agent (car) is allowed to perform stochastic actions defined as lotteries on the set of possible actions.
We consider two variants for solving the problem. In the first variant we consider only pure policies, while in the second variant we consider slightly extended mixed policies. In the second approach the size of the search space is considerably larger. For each variant we firstly consider a purely sequential implementation, that is very inefficient because of the high computational cost required by the GA. Therefore, we also investigate improved versions of our approach by employing parallel approaches to GA.
We present some of the experimental results that we obtained with our implementations. We compare these experimental results we those obtained previously using Q-learning and SARSA algorithms. This allows us to highlight the challenges and limitations of the application of GA for solving the MCP.

A Review on Algorithmic Extensions and Convergence Theory for Randomized Kaczmarz Iteration Methods

Z. Bai

We consider the iterative solution of the large and sparse system of linear equations

$$Ax = b, \quad \text{with} \quad A \in \mathbb{C}^{m\times n} \quad \text{and} \quad b \in \mathbb{C}^m. \tag{1}$$

When the matrix $A \in \mathbb{C}^{m\times n}$ is huge and impossible to be stored in a whole in the computer memory, the frequently used and also the only possible approach for computing an approximate solution to the linear system (1) may be the iteration methods that allow to use only a small part of the data from the matrix A.
In this paper, we are going to review and compare two classes of the state-of-the-art randomized orthogonal projection iteration methods based on the Kaczmarz method and the *coordinate descent* (**CD**) method. The first class is the randomized Kaczmarz-type methods, typical representatives include the *randomized Kaczmarz* (**RK**) method, the *greedy randomized Kaczmarz* (**GRK**) method, the *randomized extended Kaczmarz* (**REK**) method, the *partially randomized extended Kaczmarz* (**PREK**) method, and the *greedy randomized augmented Kaczmarz* (**GRAK**) method; and the second class is the randomized coordinate-descent-type methods, typical representatives include the *randomized coordinate descent* (**RCD**) method, the *greedy randomized coordinate descent* (**GRCD**) method, and the *randomized extended Gauss-Seidel* (**REGS**) method. For these iteration methods, by classifying the linear system (1) according to the four cases: consistent with full column-rank (Case (a)), consistent with deficient column-rank (Case (b)), inconsistent with full column-rank (Case (c)), and inconsistent with deficient column-rank (Case (d)), we deeply anatomize and highly purify their asymptotic convergence properties. In addition, based on detailed discussions we comment and summarize their advantages and disadvantages in terms of both theory and computations, when they are used to solve either the consistent or the inconsistent linear systems of the form (1).

Parametric Analysis of Space-Time Fractional Pennes Bioheat Model Using a Collocation Method Based on Radial Basis Functions and Chebyshev Polynomials

H. Bansu, S. Margenov

In this talk, space-time fractional Pennes bioheat model with sinusoidal heat flux condition on skin tissue is considered in Caputo sense. The model involves parameters like blood perfusion rate, specific heat, thermal conductivity, heating frequency etc. The numerical solution of the fractional bioheat model is obtained using a collocation method. The method involves a Kronecker product of two different basis functions, namely radial basis functions and Chebyshev polynomials.
The heat transfer process in skin tissue is studied under the influence of space-time fractional derivatives using the presented model. Temperature profiles are obtained along time and distance for different order fractional derivatives. The effect of various parameters, like heating frequency and thermal conductivity, on the heat transfer process is examined under fractional derivatives.

Accelerated Quasi-Newton Schemes For Multiphysics Problems

N. A. Barnafi

Quasi-Newton methods is a rather loose term, used to refer to any variant of a Newton method in which the Jacobian matrix is modified. This is done in order to obtain a method that converges in more iterations, but where the inversion of the (approximated) Jacobian is much faster. In this presentation, we will show some block-partitioned strategies where the components of the Jacobian can be lagged to the residual through the iterations. This yields, on one hand, an approximated Jacobian whose preconditioner is much better than the one known for the original one, but on the other hand the iteration count will be much higher. This increase in nonlinear iterations can be alleviated by using Anderson acceleration, which enjoys many theoretical properties that make it a desirable accelerator.
This approach is best understood in the framework of nonlinear preconditioners. The resulting scheme will be simply an Anderson accelerated Richardson scheme, where each iteration is preconditioned by the action of the inverse of the approximate Jacobian. We highlight this step, because the action of the Jacobian inverse can be represented by the solution of a linear system by means of, i.e. a preconditioned GMRES iterative method, but it can also be approximated simply by the action of the preconditioner. This shows that the action of the iterative linear solver can be sometimes discarded, in favor of reducing computational time, as well as keeping reducing the overall complexity in parameters that our methods require.
The resulting nonlinear scheme will be balanced in terms of who does what: the preconditioner is optimal for the approximate Jacobian, and the nonlinear terms that are lagged to the residual are adequately handled by the acceleration scheme. We will show how this can yield not only significant reductions in computational time, but also a more robust solver. These claims will be validated by numerous numerical tests in different physical contexts.

Nitsche's and Mixed Formulations of Frictionless Contact-Mechanics for Mixed-Dimensional Poromechanical Models

L. Beaude, F. Chouly, M. Laaziri, R. Masson

In this work, we address the discretization of single-phase Darcy flows in a fractured and deformable porous medium, including frictional contact at the matrix-fracture interfaces. Fractures are described as a network of planar surfaces leading to the so-called mixed or hybrid-dimensional models. Small displacements and a linear elastic behavior are considered for the matrix. To simulate the coupled model, we employ a Hybrid Finite Volume scheme for the flow and we investigate two different formulations of the contact mechanics. First, we consider a mixed discretization combining a $\mathbb{P}_2$ Finite Element conforming discretization for the mechanical displacement with face-wise constant Lagrange multipliers along the fractures, representing normal and tangential stresses [Bonaldi et al, JCP 2022]. Second, we investigate Nitsche's method [Chouly et al 2013] that involves only the displacement variables and therefore do not require any discrete inf-sup condition between the displacement and Lagrange multiplier discrete spaces unlike the mixed methods. A variant of The Nistche's method is also investigated both theoretically and numerically which is shown to match the mixed formulation with piecewise constant Lagrange multipliers at the limit of large stabilization parameters. These numerical methods are compared in terms of accuracy and robustness on several test cases.

Efficient Solution of Stochastic Galerkin Matrix Equations via Reduced Basis and Tensor Train Approximation

M. Béreš

The focus of this contribution is the development of a computational method for efficiently solving matrix equations arising from the stochastic Galerkin discretization of steady Darcy flow problems with uncertain, sepa- rable permeability fields. The proposed method involves a two-step solution process. In the first step, a reduced basis is constructed for the finite element (FE) portion of the discretization using the Monte Carlo (MC) method. Var- ious sampling techniques for the MC method are considered. In the second step, a tensor polynomial basis is employed to handle the stochastic part of the problem, and a tensor-train (TT) approximation is used to approximate the overall solution of the reduced SGM system. To improve the convergence of the TT approximation, an implicitly preconditioned system is employed, with a Kronecker-type preconditioner. Additionally, this paper includes the development of cheap error indicators for assessing the accuracy of both the reduced basis and the final solution of the reduced system.

AMG Preconditioned Communication-Avoiding Conjugate Gradient for Multi-GPU Systems

M. Bernaschi, M. Carrozzo, A. Celestini, P. D'Ambra, F. Vella

In computational and data science applications, solving sparse and large linear systems is a common and time-consuming task. Therefore, a significant amount of effort is being dedicated to designing and developing accurate and efficient iterative linear solvers able to exploit modern hybrid supercomputers. Preconditioned Conjugate Gradient (CG) is the method of choice to solve symmetric positive-definite linear systems. However, the parallel implementation of the classic CG method is limited by the high cost of communication and global synchronization, as demonstrated by the low efficiency achieved by the High-Performance CG (HPCG) benchmark, even on Top-500 supercomputers.

We discuss our recent activities in developing a version of the well known s-step preconditioned Conjugate Gradient method (Chronopoulos and Gear, 1989) for large clusters of hybrid nodes leveraging GPU accelerators. The s-step formulation of CG, recently referred as Communication Avoiding CG (CA-CG), is based on the idea of performing iterations in blocks of s, by computing $\mathcal{O}(s)-$dimensional Krylov subspace basis at each step so that s new vector solutions can be obtained from this subspace. In this way, global synchronization costs are reduced by a factor of $\mathcal{O}(s)$, improving the scalability features of the method.

One of the main challenges in the development of preconditoned CA-CG is to balance the spectral properties of the preconditioner and its intrinsic parallelism while ensuring that there is no significant penalization in terms of convergence as the system size increases. We focus on using highly-parallel AMG preconditioners to efficiently exploit GPU acceleration both in the setup and in the application phase. Thus, our methods and implementations aim to combine communication-avoiding techniques, fine-grained parallelism, and overlapping between computation and data communication to obtain a scalable linear solver. We aim to release a reliable solver that can handle large and sparse systems with high efficiency.

Characterization of Filippov Representable Maps and Clarke Subdifferentials

M. Bivas, A. Daniilidis, M. Quincampoix

The ordinary differential equation $\dot{x}(t) = f(x(t)),\ t \geq 0$, for f measurable, is not sufficiently regular to guarantee existence of local solutions. To remedy this we may relax the problem by replacing the function f with its Filippov regularization F_f and consider the differential inclusion $\dot{x}(t) \in F_f(x(t))$ which always has a local solution. It is interesting to know, inversely, when a set-valued map Φ can be obtained as the Filippov regularization of a (single-valued, measurable) function. In this talk we give a full characterization of such set-valued maps, hereby called Filippov representable. This characterization also yields an elegant description of those maps that are Clarke subdifferentials of a Lipschitz function.

Reduced Order Methods for Parametric Eigenvalue Problems

D. Boffi

Reduced order methods are consolidated and effective tools for the numerical approximation of parametric partial differential equations.
Several new challenges show up for the approximation of parametric PDE eigenvalue problems. The main difficulties are related to the possible degeneracy of the problem in presence of clusters of eigenvalues that can lead to crossings and singularities of the solutions.
At the moment when we started our investigations, the application of reduced order models to eigenvalue problems was well understood only in very particular cases, while several questions remain open.
In this talk I will review the state of the art, discuss some critical cases, and show how to deal with them. A crucial aspect consists in the capability of tracking the eigensolutions and to detect their behavior when intersections occur.

The Rough Hawkes Heston Stochastic Volatility Model

A. Bondi, S. Pulido, S. Scotti

We study an extension of the Heston stochastic volatility model that incorporates rough volatility and jump clustering phenomena. In our model, named the rough Hawkes Heston stochastic volatility model, the spot variance is a rough Hawkes-type process proportional to the intensity process of the jump component appearing in the dynamics of the spot variance itself and the log returns. The model belongs to the class of affine Volterra models. In particular, the Fourier-Laplace transform of the log returns and the square of the volatility index can be computed explicitly in terms of solutions of deterministic Riccati-Volterra equations, which can be efficiently approximated using a multi-factor approximation technique. We calibrate a parsimonious specification of our model characterized by a power kernel and an exponential law for the jumps. We show that our parsimonious setup is able to simultaneously capture, with a high precision, the behavior of the implied volatility smile for both S&P 500 and VIX options. In particular, we observe that in our setting the usual shift in the implied volatility of VIX options is explained by a very low value of the power in the kernel. Our findings demonstrate the relevance, under an affine framework, of rough volatility and self-exciting jumps in order to capture the joint evolution of the S&P 500 and VIX.

Multilevel Methods for Nearly-Singular Problems in Mixed Dimensions

A. Budiša, X. Hu, M. Kuchta, K.-A. Mardal, L. T. Zikatanov

We consider nearly singular problems, that is, problems with operators that are small, but non-singular perturbations of singular operators. Discretizations of such problems lead to matrices with condition numbers of the system growing rapidly with mesh size and model parameters.

This results in slow convergence even when using preconditioners which are optimal when the nonsingular perturbation dominates. To design efficient preconditioners we follow the theory of the method of subspace corrections and construct block Schwarz smoothers for the underlying multilevel solution method. The blocks are chosen specifically to cover the supports of the vectors/functions spanning the kernel of the singular part of the operator. We demonstrate key features of such solvers on a mixed-dimensional model of electrodiffusion in brain tissue.

An a Posteriori Error Estimator for the Spectral Fractional Power of the Laplacian

R. Bulle, O. Barrera, S. P. A. Bordas, F. Chouly, J. S. Hale

Fractional powers of the Laplacian operator are important tools in the modeling and study of non-local phenomena. Several numerical challenges arise from the discretization of these operators due to their non-local nature. For example, a direct discretization via finite element methods can lead to dense and possibly large linear systems. One way to circumvent this density is by using a rational scheme combined with a finite element method.
In this talk we describe a novel local a posteriori estimator for the finite element discretization error measured in the L2 norm that can be used to perform adaptive mesh refinement. This estimator is adapted from the strategy introduced by Bank and Weiser and can be used with any rational approx- imation scheme such as best uniform rational approximations or schemes based on the Dunford–Taylor formula. Especially, our estimator preserves the locality and robustness of the Bank–Weiser estimator and preserves the parallel nature of rational approximations. In addition, oour method can be combined with an estimator for the rational approximation error to obtain a more complete description of the discretization errors.
Finally, we use an implementation in the FEniCSx finite element software to demonstrate the performances of our method on several numerical experiments including three–dimensional problems.

A System of Hamilton-Jacobi Equations Characterizing Geodesic Centroidal Tessellations

F. Camilli, A. Festa

We introduce a class of systems of Hamilton-Jacobi equations characterizing geodesic centroidal tessellations, i.e. tessellations of domains with respect to geodesic distances where generators and centroids coincide. Typical examples are given by geodesic centroidal Voronoi tessellations and geodesic centroidal power diagrams. An appropriate numerical scheme on unstructured grids allows computing the solution of the Hamilton-Jacobi system and therefore the associated tessellations. We discuss various numerical examples to illustrate the features of the technique.

Computing the Mittag-Leffler Function of a Matrix Argument

J. R. Cardoso

It is well-known that the two-parameter Mittag-Leffler function plays a key role in Fractional Calculus. In this talk, we address the problem of computing this function, when its argument is a square matrix. Effective methods for solving this problem involve the computation of successive derivatives or require the use of mixed precision arithmetic. We provide an alternative method that is derivative-free and can work entirely using IEEE standard double precision arithmetic. Theoretical and numerical issues regarding the performance of the method are investigated. A set of numerical experiments show that our novel approach is competitive with the existing ones, in terms of accuracy and computational cost.

Mixed Finite Element Methods for Fluid-Poroelastic Structure Interaction

S. Caucao, T. Li, I. Yotov

The Stokes-Biot model describes the interaction between a free fluid and a fluid in a poroelastic material. The two regions are coupled via suitable interface conditions, including balance of forces, continuity of normal velocity, and no-slip or slip with friction tangential velocity condition. We develop a fully mixed formulation for the Stokes-Biot model. It is based on weakly symmetric deviatoric stress, velocity, and vorticity for Stokes, weakly symmetric stress, displacement, and rotation for elasticity, and mixed velocity and pressure for Darcy flow. This formulation exhibits multiple advantages, including local conservation of mass for the Darcy fluid, local poroelastic and Stokes momentum conservation, accurate approximations with continuous normal components for the Darcy velocity, the poroelastic stress, and the free fluid stress, locking-free behavior, and robustness with respect to the physical parameters. Well posedness of the variational formulation and its mixed finite element approximation is established. Stability and error analysis is performed for the numerical method. Furthermore, we employ a multipoint stress mixed finite element method for the discretization of the Stokes and elasticity equations, as well as a multipoint flux mixed finite element method for the Darcy flow. The method allows for local elimination of the stresses, Darcy velocity, vorticity, and rotation, resulting in a symmetric and positive definite cell centered system involving only the Stokes velocity, displacement, and Darcy pressure. Numerical results are presented to illustrate the performance of the method, including its flexibility and robustness for several geoscience applications.

Parallel Solution of the Schrödinger-Poisson Equation on GPUs

J. Cervenka, R. Kosik, F. Ribeiro

Quantum mechanical effects exhibited in carrier transport must often be accounted for in the development of future electronic devices. To achieve physically reasonable results, the transport

equation of the quantum mechanical system and the electrical problem (Poisson equation) have to be solved self-consistently.
Due to the high computational costs of the solving mechanism, however, a parallelization of the procedure is essential in order for simulation results to be obtained in a time frame acceptable to a device engineer.
In the used technique the Newton method has to be applied on a coupled Schrödinger-Poisson system for each bias point, requiring the assembly of the Jacobian with respect to the unknowns. Here, the number of Schrödinger equations to be solved during the assembly of the Jacobian scales with the product of the number of points in the spatial grid and in k-space. In a typical simulation this requires several millions of Schrödinger-type equations to be solved for the assembly of the Jacobian.
The problem structure shows a variety of similar independent calculations which is feasible for parallelization and transferable to GPUs. Special care has to be taken because of the memory limitation of the GPU. To prevent a parallel storage of the system matrices, the discretization is carried out by a reformulation of the problem in terms of one-sided boundary conditions. An explicit scheme can be employed and no individual system matrices need to be assembled.
For the implementation we rely on the CUDA platform. Simulations are carried out on general purpose GPUs. Traditional CPUs are utilized for reference. Benchmarks demonstrate a scalability of up to several thousands of calculations in parallel.

Clouds Formed by Thermals Arising and Evolving under the Influence of the Coriolis Force

H. Chervenkov, V. Spiridonov

In the presented study mushroom-like cloud structure in the atmosphere of the Northern Hemisphere has been studied. Examples of such a structure are shown and compared with the result of a simple analytical model of thermals developing in a gravitational field. This structure can be described as a consequence of the action of the Coriolis force at a certain degree of atmospheric instability. The conditions for the occurrence and development of single thermal have been analyzed. For this purpose, the parcel theory of a thermal formation is utilized. The studied cloud structures are relatively rare, which makes it difficult to determine the conditions for their appearance. These structures are mostly observed in the cool part of the year. Subsequently, the contrast between the temperature in the tropical part of the ocean and that in the polar regions favors the occurrence of horizontal convection caused by the Coriolis force. It was found that the instability index, introduced by the authors in another study, should have values below minus one. The outcomes of the study suggests that there is an optimal range of temperature difference between the thermals and environment as well as suitable wind and a level of instability for the development of the considered phenomena.

Extending Rademacher Theorem to Set-Valued Maps

A. Daniilidis, M. Quincampoix

Rademacher theorem asserts that Lipschitz continuous functions between Euclidean spaces are differentiable almost everywhere. In this work we extend this result to set-valued maps using an adequate notion of set-valued differentiability relating to convex processes. Our approach uses Rademacher theorem but also recovers it as a special case.

Anastylosis of Frescos - a Web Service in an HPC Environment

D. T. Dimov, T. Gurov, S. Ivanovska, S. Yordanov

Anastylosis of Frescos, or virtual restoration of frescoes from their ruins, is the application area of the so-called RINCCAS method (Rotation-Invariant Normalized Cross-Correlation (NCC) method for 2D color matching of Arbitrary Shaped fragments) that was initially developed at IICT-BAS for participation in DAFNE (Digital Anastylosis of Frescos challeNgE) computer competition, June-July 2019. The fresco is expected to be represented by a painting or sketch relatively well preserved over time. The fragments collected from the ruins, of random shapes and sizes, possibly mixed with other, spurious fragments, are also expected to be given by their images. This problem statement is well known in the practice of World Heritage conservation. RINCCAS method consists of 2 phases: Phase-1 has is cubic complexity and requires significant computational resources, even with relatively small input data. Phase-2 recognizes false fragments with linear complexity based on the precise virtual positioning of all fragments.
In this work we present RINCCAS-HPC web service which accelerates Phase-1 by using the Avitohol supercomputer in IICT-BAS. The proposed paper describes and discusses:

1. Briefly the original method, algorithm and program code of RINCCAS: MACIR innovations and acceleration by data scaling; rotational independence of NCC, and the processing complexity.
2. The proposed RINCCAS parallelization scheme and its optimal adaptation to used resource of the Avitohol supercomputer.
3. The numerical results using the above HPC system to accelerate anastylosis with data from the DAFNE database and the improved complexity.
4. The features the RINCCAS-HPC web service, where both phases of RINCCAS method are included.
5. Directions for future work.

Logical Qubit Implementation for Quantum Annealing

H. Djidjev

Using quantum annealers for solving large optimization problems such as computing Boolean tensor networks, scheduling, and portfolio optimization requires embedding of the logical structure of the problem into the structure of the quantum device. For this end, each variable of the

problem has usually to be represented by a connected set of qubits called a logical qubit or a chain. To force all the physical qubits in a chain to take the same value in a solution proposed by the annealer, a ferromagnetic coupling (negative weight) between the chain qubits is applied. Finding an appropriate weight value is crucial for the ability of quantum annealing to solve the resulting problem. If the magnitude of the weight is too low, the physical qubits may not take the same value, rendering such solution invalid. If it is too high, it results in ill-conditioning and a loss of precision. This work proposes an optimization-based approach based on the augmented Lagrangian method for producing suitable logical qubits representations. Experiments on the D-Wave Advantage system for solving the maximum clique problem on random graphs show that the proposed approach outperforms, with respect to the accuracy of the obtained solution, both the widely used default D-Wave method for chain-weight assignment and the quadratic penalty method.

A Posteriori Error Estimates for Hybrid High-Order Methods on Polygonal and Polyhedral Meshes

Z. Dong, A. Ern, G. Pichot

We present a new residual-type energy-norm a posteriori error analysis for hybrid high-order (HHO) methods for elliptic problems. The new error bounds are also applicable to HHO methods on meshes consisting of elements with very general polygonal/polyhedral shapes. The case of simplicial and/or box-type elements is included in the analysis as a special case. In particular, for the upper bounds, an arbitrary number of very small faces are allowed on each polygonal/polyhedral element as long as certain mild shape regularity assumptions are satisfied, which is essential for designing the adaptive algorithms based on the mesh agglomeration strategy for large-scale simulations. As a corollary, the present analysis holds for meshes with an arbitrary number of irregular hanging nodes per element. The proof hinges on a new conforming recovery strategy in conjunction with a Helmholtz decomposition formula. Local lower bounds are also proven for a number of practical cases. Numerical experiments are also presented, highlighting the practical value of the derived a posteriori error bounds as error estimators and also the flexibility of the adaptive algorithms based on the mesh agglomeration.

Solving Equations with Fractional Powers of Elliptic Operators by Padé Approximation

B. Duan, R. Lazarov, J. Pasciak

The purpose of the talk is to derive and theoretically justify an approximation method for solving the equation $\mathcal{A}^\alpha u = f$. Here $\mathcal{A}$ is a self-adjoint and coercive elliptic operator defined on a dense subset of $L^2(\mathcal{M})$ and $0 < \alpha < 1$. Here $\mathcal{M}$ could be a bounded Lipschitz domain in $\mathcal{R}^n$, $n = 2, 3$, or a certain 2-D manifold and the fractional power of $\mathcal{A}$ is defined through its spectrum.

In applications such problems are discretized by a finite difference or finite element method on a mesh with a step-size h leading to an algebraic system $\mathcal{A}_h^\alpha u_h = f_h$ for $u_h \in \mathcal{R}^N$ with

$\dim \mathcal{R} = O(h^{-n})$. For solving such large systems desirable are methods that are robust with respect to $\alpha \in [0,1]$.
Due to Vabishchevich, $u_h = \tilde{u}_h(1)$, where $\tilde{u}_h(t)$ is a solution of the initial value problem $(\delta\mathcal{I} + t\mathcal{B}_h)\partial_t\tilde{u}_h(t) + \alpha\mathcal{B}_h\tilde{u}_h(t) = 0,\ t \in (0,1],\ \tilde{u}_h(0) = \delta^{-\alpha}f_h$, and $\mathcal{B}_h = \mathcal{A}_h - \delta\mathcal{I}$. Here δ a bound from below of the spectrum of $\mathcal{A}_h$ and $\mathcal{I}$ is the identity operator. We propose to approximately solve this problem on a geometrically graded near $t = 0$ mesh $0 = t_0 < t_1 < \cdots < t_{L+1}$. On each time-step t_j we use a diagonal Padé approximation $P_m(t)/Q_m(t)$ of $(1+t)^{-\alpha}$ on $[0,1]$ to produce a $U_{L+1} \approx \tilde{u}_h(1)$. This algorithm results in solving m systems of the type $(\delta\mathcal{I} + t_j\mathcal{B}_h)v = g$, $j = 1, 2, \ldots, L+1$, so that the complexity of the method is roughly $m(L+1)$ inversions of $\mathcal{A}_h$. Our main results is: *the Padé approximate solution U_{L+1} is exponentially convergent to u_h*, namely, $\|u_h - U_{L+1}\|_{L_2} \le c\delta^{-\alpha}2^{-5m}\|f_h\|_{L_2}$ with a constant c that is independent of h, L, and m. The theoretical convergence rate is justified by numerical experiments on a number of test problems.

Cell-Based Modeling and Simulation of Electrical and Chemical Interplay in Excitable Tissue

A. J. Ellingsrud, R. Masri, M. Kuchta

Today, the classical homogenized models for simulating excitable tissue are challenged by new mathematical frameworks that explicitly represent and resolve the geometry of extracellular and intracellular spaces and cellular membranes (EMI models). These mixed-dimensional models crucially enable an abstract representation of heterogeneous distributions of membrane ion channels and realistic cellular morphologies. EMI models typically predict the electrical properties of the tissue, with the underlying assumption that the ion concentrations are constant. Although the resulting models give accurate predictions of neuronal electrodynamics in many scenarios, they fail in capturing the numerous phenomena related to shifts in the extracellular ion concentrations.
Here, we discuss an alternative approach to detailed modeling of excitable tissue that also accounts for ion concentration dynamics. In particular, we consider a mathematical model describing the distribution and evolution of ion concentrations and electrical potentials. The model defines a non-linear and mixed-dimensional PDE system coupling the unknown fields defined over cellular domains and fields defined over the lower-dimensional cellular membranes. As a combination of the electroneutral Kirchhoff-Nernst-Planck (KNP) model and the EMI framework, we refer to this model as the KNP-EMI model. We introduce and evaluate a new, finite element-based numerical scheme for the KNP-EMI model, capable of efficiently and flexibly handling geometries of arbitrary dimension. Specifically, we eliminate the unknown fields defined over the lower-dimensional membranes to obtain a single-dimensional problem, apply a splitting scheme and discretize the separate subproblems using a DG finite element method. We discuss stability and convergence properties of the proposed scheme. Finally, we compare the electrical potentials predicted by the KNP-EMI and EMI models and study ephaptic coupling induced in an unmyelinated axon bundle and demonstrate how the KNP-EMI framework can give new insights in this setting.

Towards Efficient SOT-assisted STT-MRAM Cell Switching using Reinforcement Learning

J. Ender, R. Lacerda de Orio, W. Goes, V. Sverdlov

Nonvolatile memory is a promising candidate to replace CMOS devices. The two most common magnetoresistive RAM (MRAM) cell types use the so-called spin-transfer torque (STT) and spin-orbit torque (SOT) to write information into the memory cell. Each of these has its drawbacks, STT-MRAM suffers from oxide degradation due to high write current densities, SOT-MRAM requires additional symmetry-breaking measures for reliable switching of the magnetization. This has led researchers to apply both of these methods in a single memory cell. The two methods, each compensating the drawback of the other, complement each other perfectly. Besides the growing interest in nonvolatile memories like MRAM, machine learning algorithms have gained massive interest and are penetrating all possible scientific domains, often achieving staggering results. The machine learning subfield of reinforcement learning (RL) gained popularity when first applied to computer and board games, but has since proven helpful in many other disciplines. It enables a virtual agent to learn how to optimally interact with an environment to achieve a certain goal, by rewarding or punishing it for performed actions.
We developed an approach, in which we train an RL agent to learn how to switch such a hybrid SOT-assisted STT-MRAM cell, allowing it to apply STT and SOT current pulses independently. During this process the agent is encouraged to reverse the magnetization in the memory cell fast and by using little energy. After successfully training the RL agent to reverse the magnetization in SOT-assisted STT-MRAM cells under the given constraints, we test its robustness. The environment part of the computational RL framework consists of a micromagnetic finite difference simulator written in C++ which solves the Landau-Lifshitz-Gilbert equation. This interacts with the actual training code written in Python, which is based on the RL library `stable-baselines3`.

Matrix-Based Redistribution for Improved Coarse Level Scaling in Multilevel Markov Chain Monte Carlo

H. R. Fairbanks, P. Vassilevski

Scalable approaches for performing Bayesian inference are necessary for characterizing prediction confidence in large-scale PDEs with random coefficients. Many approaches to perform Bayesian inference in this setting are too expensive, e.g., Markov chain Monte Carlo (MCMC). With the increase in problem size and thus high-fidelity (fine grid) simulation cost, MCMC becomes intractable, and acceleration approaches become necessary.
One acceleration approach to consider is multilevel MCMC, which accelerates the estimation of fine grid statistical quantities of interest by exploiting a hierarchy of coarse grid (level) discretizations of partial differential equations (PDEs). However current implementations are not suitable to large-scale problems, as the random coefficients are not generated in a scalable manner.
In recent work, we developed an algorithmically scalable PDE-based sampling method to generate random coefficient realizations on each level of the multilevel MCMC hierarchy. This was

done by using scalable algebraic multigrid methods used in the PDE-sampling. A shortcoming of this approach was that it was not fully scalable due to restrictions on the parallel coarse grids. While this approach demonstrated algorithmic scaling on all levels, full simulation scaling was not achieved across all levels, as the mesh on each level was distributed across the same number of processors.
To attain full simulation scaling, we exploit an element agglomerated coarsening based on redistributing data to a reduced number of processors, which ensures both guaranteed coarse level accuracy and improves the solver scalability on coarse levels. The proposed redistribution utilizes only parallel sparse-matrix operations. This is completed during the AMG hierarchy construction to easily incorporate redistribution into multilevel MCMC. In this presentation, we will provide a high-level overview of our PDE-based random coefficient sampling approach used for multilevel MCMC, the newly developed redistribution method, and provide numerical examples to show improvements in coarse grid scaling.

Nonstandard Finite Difference Method and its Application to Epidemic Propagation

I. Faragó

We consider the dicretization of the Cauchy problem for the equation $u' = f(u)$ with $u(0) = u_0$. Our aim is construct such discrete models which result in convergent numerical solutions, and the discrete solutions preserve the main qualitaive properties of the solution of the continuous model.
As it is known, the explicit Runge–Kutta (ERK) methods are insufficient methods for stiff problems, due to lack of A-stability. Moreover, they preserve the nonnegativity only conditionally. These features make them ineffective for dealing with dynamical systems, which are frequently studied over very large time periods. In our talk for the discretization we use the combination of an ERK method with the nonstandard finite difference (NSFD) method. We show that this combined method does not only preserve the consistency order and convergence of the base ERK method but also have many other good features: it is both absolute stable and unconditionally nonnegativity preserving. We demonstrate our theoretical results on the extended Ross model for malaria propagation:

$$\begin{aligned}
\dot{S}_h(t) =& \Lambda_h - \frac{b\beta_h S_h(t) I_m(t)}{1+\nu_h I_m(t)} - \mu_h S_h(t) + \omega R_h(t);\\
\dot{E}_h(t) =& \frac{b\beta_h S_h(t) I_m(t)}{1+\nu_h I_m(t)} - (\alpha_h + \mu_h) E_h(t);\\
\dot{I}_h(t) =& \alpha_h E_h(t) - (r + \mu_h + \delta_h) I_h(t);\\
\dot{R}_h(t) =& r I_h(t) - (\mu_h + \omega) R_h(t);\\
\dot{S}_m(t) =& \Lambda_m - \frac{b\beta_m S_m(t) I_h(t)}{1+\nu_m I_h(t)} - \mu_m S_m(t);\\
\dot{E}_m(t) =& \frac{b\beta_m S_m(t) I_h(t)}{1+\nu_m I_h(t)} - (\alpha_m + \mu_m) E_m(t);\\
\dot{I}_m(t) =& \alpha_m E_m(t) - (\mu_m + \delta_m) I_m(t),
\end{aligned}$$

with given intial condition at $t = 0$.

Mean Field Games in Infinite Dimension

S. Federico, D. Ghilli, F. Gozzi

The theory of Mean Field Games has experienced in the last 15 years a huge attention of the mathematical community. Developed starting from seminal papers by Lasry and Lions (2007) and Huang, Malhame, and Caines (2006), it represents an elegant way to describe dynamic games with a large but symmetric number of players. Several applications ranging in a wide variety of fields (including Economics and Finance) have been provided relying upon this mathematical framework, as well as monographs at a theoretical and applied level appeared. By the way, the literature of infinite-dimensional mean-field games is still basically missing — with the exception of a copule of papers dealing with very specific problems (see below). This is somehow surprising, as the mathematical technology to treat *separately* the infinite-dimensional equations of the mean-field game problem (that is, the Hamilton Jacobi-Bellman and the Fokker-Plank equation) is already existing. Our aim is to fill this gap, that is, relying on the available results – in infinite dimension – on these equations in separate form, to merge them in order to get results on the coupled system in the spirit of the finite dimensional theory of mean-field games. We provide some results in the Linear-Quadratic case and describe some ideas on how to treat more general structures. The aim is also to provide examples of application arising in Finance/Banking (systemic risk) and Economics (vintage capital).

Ant Algorithm with Local Search Procedure for Multiple Knapsack Problem

S. Fidanova, K. Atanassov

Multiple Knapsack Problem (MKP) is a hard combinatorial optimization problem with large application. A lot of real life and industrial problems can be defined like MKP, therefore it attracts the attention of the scientists. Exact methods and traditional numerical methods are appropriate for solving small problems or problems without hard constraints. For problems, which needs non polynomial (NP) number of calculations is better to apply so called metaheuristic methods. Metaheuristics are methodology and on their basis is constructed problem dependent algorithm. Metaheuristic methods apply some stochastic rules and it helps to find faster near optimal solution even for huge problems. Ant Colony Optimization (ACO) is a nature inspired method, which follows the real ants behavior. It is between the best methods for solving combinatorial optimization problems. It is population based, agent based method, which is based on indirect communication between the agents with the help of distributed numerical information, called pheromone, with analogy of real ants. The pheromone information is used for probabilistic construction of solutions. The pheromone is adapted during the execution of the algorithm to reflect ants experience in solution construction. Sometimes the method alone is not enough to find good solutions, especially when the problem has strong constraints. In this case, one resorts to constructing an appropriate local search procedure. The aim is to find better solutions or to fasten the search process. MKP is a subset problem. There is a set of objects with some profit and we try to select part of them, thus to have subset with highest possible profit respecting the constraints of the problem. The solutions of the problem can be represented by binary sequence. Let us consider this binary sequence as a binary number. We

will calculate the average between the best solution, represented as a binary number, and any of the current solutions. The new binary number will be the new solution after local search procedure.

Machine Learning Algorithms for Parameter Identification of Reactive Flow in Porous Media

D. Fokina, V. Grigoriev, O. Iliev, I. Oseledets

Reactive flow through porous media processes are present in many industrial and environmental systems and a better understanding of these processes may improve the control over such systems. In this work we study the pore scale species transport in presence of surface (heterogeneous) reactions of adsorption and desorption. The transport of species is modeled by a convection-diffusion equation, the flow is described by incompressible Stokes equations. The surface kinetics is included via Robin boundary conditions. We are interested in identifying the reaction coefficients, i.e. in solving an inverse parameter identification problem. Solving the inverse problem requires solving the direct problem many times (e.g. thousands). The extra information which is used to solve the parameter identification problem is the outlet concentrations, so-called breakthrough curves. These curves can be well approximated using machine learning algorithms. Replacing the numerical solution of the direct problem with a machine learning model significantly speeds up computational times. Recently we have shown that machine learning models can well approximate the breakthrough curves in the case of homogeneous reactions. In this presentation we consider parameter identification for heterogeneous reactions using several numerical solutions to train the machine learning model and then use them to generate new curves, required to identify the parameters. We consider several machine learning methods and discuss the results of each of them.

Simulation of Reactive Flow in Fractured Porous Media with Hybrid Dimensional Models and Polytopal Grids

L. Formaggia, A. Fumagalli, A. Scotti

Geochemical reactions, particularly dissolution/precipitation phenomena, may affect the underground flow considerably because of the induced porosity and permeability variations. The situation is even more critical in the presence of fractures since their presence may provide a preferential pattern for the solute. In this work, we simulate the coupled fluido-thermo-chemical problem using a hybrid dimensional discretization scheme where we model the fractures as a network of immersed one-codimensional manifolds. We use a simple yet representative dissolution/precipitation model in the rock matrix and fracture network. To increase the geometrical flexibility, we employ numerical schemes operating on general polytopal meshes and based on virtual element and finite volume methodologies.

Minimization of Energy Functionals via FEM: Implementation of hp-FEM

M. Frost, A. Moskovka, J. Valdman

Many problems in science and engineering can be rigorously recast into minimizing a suitable energy functional. We have been developing efficient and flexible solution strategies to tackle various minimization problems by employing finite element discretization with P1 triangular elements [1,2]. An extension to rectangular hp-finite elements in 2D is introduced in this contribution.

A Machine Learning Technique for the Darcy Problem in a Fractured Porous Media that Esure Local Mass Conservation

A. Fumagalli, W. M. Boon

Constructing fast solution schemes often involves deciding which errors are acceptable and which approximations can be made for the sake of computational efficiency. Herein, we consider a mixed formulation of Darcy flow and take the perspective that the physical law of mass conservation is significantly more important than the constitutive relationship, i.e. Darcy's law. Within this point of view, we propose a three-step solution technique that guarantees local mass conservation.
In the first step, an initial flux field is obtained by using a locally conservative method, such as the TPFA Finite Volume Method. Although this scheme is computationally efficient, it lacks consistency and therefore requires a suitable correction. Since this correction is divergence-free, the Helmholtz decomposition ensures that it is given by the curl of a potential field. The second step therefore employs an H(curl)-conforming discretization to compute the correction potential and update the flux field. The pressure field is computed in the final step by using the same TPFA system from the first step.
The procedure guarantees local mass conservation regardless of the quality of the computed correction. Thus, we relax this computation using tools from reduced order modeling. We introduce a reduced basis method that is capable of rapidly producing a potential field for given permeability fields. By applying the curl to this field, we ensure that the correction is divergence-free and mass conservation is not impacted.
Finally, we extend the method to solving Darcy flow in fractured porous media. We rewrite the equations in terms of mixed-dimensional differential operators and identify the problem as a mixed-dimensional Darcy flow system. In turn, the proposed three-step solution procedure directly applies using the mixed-dimensional curl to ensure local mass conservation.

Influence of the Grid Resolutions on the Computer Simulated Transport and Transformation Atmospheric Composition Processes over the Territory of Bulgaria

G. Gadzhev, I. Georgieva, K. Ganev, V. Ivanov, N. Miloshev

It should be expected that the computational grid resolution will have a significant impact on the computer simulation results. Therefore, a numerical experiment is made in order to evaluate the horizontal grid resolution impact on the simulated transport and transformation atmospheric composition processes over the territory of Bulgaria. The computer simulations are performed with a set of models used worldwide - US EPA Models 3 System. Using the "nesting" capabilities of the models, a resolution of 9 km was achieved for the territory of Bulgaria, by sequentially solving the task in several consecutive, nested areas. Three cases are considered in this paper: 1: The computer simulations results from the domain with a horizontal resolution (both of the emission source description and the grid) of 27 km; 2: The computer simulations results from the domain with a horizontal resolution (both of the emission source description and the grid) of 9 km; 3: Hybrid case with the computer simulations performed with a grid resolution of 9 km, but with emissions like in the 27x27 km domain. The simulations were performed, for all the three cases, for the period 2007 – 2014 year, thus creating an ensemble large and comprehensive enough, as to reflect the most typical atmospheric conditions with their typical recurrence. The CMAQ "Integrated process rate analysis" option is applied to obtain the spatial/temporal distribution of the different transport and transformation atmospheric composition processes. Comparing them for the above 3 cases makes it possible to evaluate the grid resolution impact.

Development of New High Performance Computer Architectures and Improvements in Danish Eulerian Model for Long Range Transport of Air Pollutants

K. Georgiev, Z. Zlatev

The paper is devoted to an analysis and comparison in the development of new high – performance computers and the improvements and development of new more reliable versions of the Danish Eulerian model for computer studying of the transport of the air pollutants over Europe and surrounding areas, studying some economical and agricultural problems, regional and global climate changing, etc.

Computation of the Unknown Time-Dependent Volatility of American Options from Integral Observations

S. G. Georgiev, L. G. Vulkov

We consider, for definiteness, the American call of the Black–Scholes model:

$$\frac{\partial C}{\partial t} = \frac{\sigma^2(t)}{2} S^2 \frac{\partial^2 C}{\partial S^2} + (r-q) S \frac{\partial C}{\partial S} - rC, \quad 0 < S < s(t),\ 0 < t < T,$$

$$C(S,0) = \max(S-K,0);\ C(0,t) = 0,\ C(s(t),t) = s(t) - K,\ \frac{\partial C}{\partial S}(s(t),t) = 1.$$

Here C is the option price, K is the strike, $\sigma(t)$ is the volatility, and r, q are the risk-free interest rate and the dividend yield, respectively, while $s(t)$ is the optimal early exercise boundary. In order to determine the unknown diffusion coefficient $\sigma^2(t)$, we impose the overdetermination condition

$$\frac{1}{s(t)} \int_0^{s(t)} C(S,t) \mathrm{d}S = \psi(t),$$

where $\psi(t)$ is a given function. Iterative numerical algorithms are proposed to solve the *inverse* problem for recovering the unknown triple $\Big(C(S,t), s(t), \sigma^2(t)\Big)$.

Evaluation of the Effects of the National Emission Reduction Strategies for Years 2020-2029 and after 2030 on the AQI on the Territory of Bulgaria

I. Georgieva, G. Gadzhev, K. Ganev, V. Ivanov, N. Miloshev

The present paper presents the results obtained in the frame of an extensive study of the effects of different emission reduction scenarios on the air quality in Bulgaria. The set of models applied for atmospheric composition simulations is the same used in the operational Bulgarian Chemical Weather Forecast and Information System. Thus, the obtained results are fully compatible with the operational chemical weather forecast. The models are also widely used in air pollution modelling, so the obtained computer simulation results are in harmony with evaluations made for other regions. Based on 3D modelling tools, an extensive database was created and used for different studies of atmospheric composition. The models in the system were adapted and validated for Bulgaria. This gave the opportunity to conduct extensive studies on a fully competitive modern level of the climate of atmospheric composition in the country. The provided model simulations are with horizontal resolution 9 kilometers for the region of Bulgaria. Complying the EU Directive 2016/2284, Bulgaria developed national emission reduction strategies for years 2020-2029 and after 2030. Evaluation of the effects of these strategies on the AQI on the territory of Bulgaria is the objective of the present study. Five emission scenarios are considered in the paper for two different periods (2020-2029 and after 2030) with existing measures (WEM) and with additional measures (WAM), and the results are compared with the reference period (2005). The basic task in the paper is getting simulated AQI on the territory

of Bulgaria. Comparing the AQI simulated with the different scenarios makes it possible to evaluate the effect of the national emission reduction strategies.

Coupled 1D-3D Network Models for Pulsatile Perivascular Fluid Flow

I. Gjerde, R. Masri, A. Poulain, M. Rognes, B. Wohlmuth

Alzheimer's disease is characterized by the accumulation of toxic proteins in the brain. According to the glymphatic theory, their removal is facilitated by CSF flow. Experimental results further indicate that CSF moves both through brain tissue and in a network of so-called perivascular spaces. The driving forces of this flow are of particular medical interest. Thus there is a need for mixed-dimensional modeling and simulation tools describing this phenomenon.
In this talk, we focus on the analysis and discretization of a time-dependent coupled 1d-3d flow model. Firstly, we present a 1D Brinkman-Stokes type network model for perivascular fluid flow. We show how the network model can be discretized using finite elements and connect the properties of the discretization to the properties of the network graph. Next, extend this to a coupled 1d-3d flow model, and discuss the well-posedness of this system. Finally, we show how the numerical simulations connect to fundamental questions in the glymphatic theory.

Generalized Convolution Quadrature For The Fractional Integral And Fractional Diffusion Equations

J. Guo, M. Lopez-Fernandez

We consider the application of the generalized Convolution Quadrature (gCQ) of the first order to approximate fractional integrals and associated fractional diffusion equations. The gCQ is a generalization of Lubich's Convolution Quadrature (CQ) which allows for variable steps. In this paper we analyze the application of the gCQ to fractional integrals, with a focus on the low regularity case. It is well known that in this situation the original CQ presents an order reduction close to the singularity. Moreover, the available theory for the gCQ does not cover this situation. Here we deduce error bounds for a general time mesh. We show first order of convergence under much weaker regularity requirements than previous results in the literature. We also prove that uniform first order convergence is achievable for a graded time mesh, which is appropriately refined close to the singularity, according to the order of the fractional integral and the regularity of the data. Then we study how to obtain full order of convergence for the application to fractional diffusion equations. For the implementation of this method, we use fast and oblivious quadrature and present several numerical experiments to illustrate our theoretical results.

A Resolvent Quasi-Monte Carlo Method for Estimating the Minimum Eigenvalues Using the Error Balancing

S.-M. Gurova, E. Atanassov, A. Karaivanova

Iterative Monte Carlo methods are used for estimating the extreme eigenvalues of large dimensional matrices. The Power Monte Carlo method allows for finding the approximate maximum and minimum eigenvalue of the considered matrix. In the case when we need to estimate the minimum eigenvalue, it is recommended to use the Resolvent Monte Carlo method. Recent developments in quasi-random sequences and their successful application motivate us to reconsider the quasi-Monte Carlo approach to eigenvalue estimation for finding the minimum eigenvalue. We propose a new algorithm that combines the Resolved Monte Carlo method with a randomized sequence that has a small discrepancy applied to an augmented symmetric matrix of arbitrary dimension. To generate this sequence we use BRODA's Sobol Randomized Sequence Generator (broda.co.uk/software.html). Numerical experiments were done that show excellent efficiency when GPU accelerators are used.

Simulation Scenarios in an Artificial Honeybee Hive

G. Haase, M. Stoiber, T. Grandits, A. Ilgün, T. Schmickl

Honeybees are important pollinators, yet many things are not really fully understood about their colony-internal integration. It is especially hard to see the "(near-)optimality" in the sheer mess of wiggling insects that "float" through a honeybee hive. Therefore, the Complexity of Life lab is going to combine observation, simulation and artificial interaction in the beehive. The hive geometry is represented by its surfaces triangles on which shortest path investigations from/to different sub-parts of the geometry are performed. Run time comparisons are presented between discrete approaches (Dijkstra algorithm and its improvement A*) and the continuous approach via the Eikonal equation [1].
Resulting from the shortest path investigations, bottlenecks in the hive design are identified resulting in potential design adjustments in the artificial bee hive of the biology lab. Additional investigations regarding evacuation scenarios might need (artificial) bee agents operating similar adapted Hughes' model in [2]. A validation of the simulations is planned in the artificial beehive at the lab.

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Solving Large-Scale Fractional Linear Systems of Sparse SPD Matrices with Small Spectrum

S. Harizanov

Consider the algebraic problem $\mathbb{A}^\alpha \mathbf{u} = \mathbf{f}$, where $\mathbb{A} \in \mathbb{R}^{n\times n}$ is a sparce, SPD matrix of large size and $\alpha \in (0,1)$. The matrix $\mathbb{A}^\alpha$ is typically everywhere dense, thus it is practically impossible to even be stored in the computer memory, let alone to perform explicit computations with it. One needs to find a cheap, but close approximation $\widetilde{\mathbf{u}}$ of $\mathbf{u}$ that also inherits important properties of the exact solution, such as non-negativity. We attack the problem via the (k,k) best uniform rational approximation (BURA) $r_{\alpha,k}(t)$ of the function t^α on the unit interval. More precisely, we define

$$r_{\alpha,k}(t) := \underset{r\in\mathcal{R}(k,k)}{\operatorname{argmin}} \|r(t) - t^\alpha\|_{C[0,1]}, \qquad E_{\alpha,k} := \|r_{\alpha,k}(t) - t^\alpha\|_{C[0,1]}.$$

In our previous works we have considered three different candidates for approximating $t^{-\alpha}$. The classical BURA approach uses $f_1(t) = r_{\alpha,k}(t^{-1})$, which is the BURA element for $t^{-\alpha}$ in the interval $[1,\infty)$. In this case, we need to normalize the spectrum of $\mathbb{A}$ in the interval above, which makes perfect sense when $\mathbb{A}$ is generated via finite element or finite difference discretizations of elliptic operators. The other two approaches approximate $t^{-\alpha}$ into the interval $(\varepsilon, 1]$, using $f_2 = t^{-1} r_{1-\alpha,k}(t)$, respectively $r^{-1}_{\alpha,k}(t)$. Here, we need to normalize the spectrum of $\mathbb{A}$ in $(\varepsilon,1]$, which works well for graph-Laplacian operators. Let the eigenvalues of $\mathbb{A}$ be $0 < \lambda_1 \le \lambda_2 \le \cdots \le \lambda_n$. Then for

$$\widetilde{\mathbf{u}}_1 := \lambda_1^{-\alpha} r_{\alpha,k}(\lambda_1 \mathbb{A}^{-1})\mathbf{f},\ \widetilde{\mathbf{u}}_2 := \lambda_n^{1-\alpha}\mathbb{A}^{-1} r_{1-\alpha,k}(\lambda_n^{-1}\mathbb{A})\mathbf{f},\ \widetilde{\mathbf{u}}_3 := \lambda_n^{-\alpha} r^{-1}_{\alpha,k}(\lambda_n^{-1}\mathbb{A})\mathbf{f}$$

the corresponding relative errors $Err_i := \|\mathbf{u} - \widetilde{\mathbf{u}}_i\|_2 / \|\mathbf{f}\|_2$ are

$$Err_1 = \lambda_1^{-\alpha} E_{\alpha,k}, \qquad Err_2 = \lambda_n^{1-\alpha}\lambda_1^{-1} E_{1-\alpha,k}, \qquad Err_3 = \lambda_n^{\alpha}\lambda_1^{-2\alpha} E_{\alpha,k}.$$

Thus, for systems where $\lambda_n \approx 1$, all the three approximations $\{\widetilde{\mathbf{u}}_i\}_{i=1}^3$ are suitable candidates, as well as affine combinations of them. In this talk we numerically investigate error minimization based on such combinations.

Rational Approximations in Robust Preconditioning of Coupled Problems

S. Harizanov, I. Lirkov, S. Margenov

Multiphysics and multiscale problems naturally involve coupling at interfaces which are manifolds of lower dimensions. Additive (block-diagonal) and multiplicative (non-overlapping domain decomposition) preconditioning of coupled stiffness matrices provide efficient approaches for numerically solving large-scale problems in this class. At the operator level, the interface blocks of the preconditioners are fractional Laplacians. At the discrete level, we replace the inverses of the fractional Laplacians with their best uniform rational approximations (BURA). In this sense the discussed preconditioners are implicitly defined.
We present a unified framework for the analysis of the discussed iterative methods. As a final result, we show that the proposed preconditioners have an optimal computational complexity

$O(N)$, where N is the number of unknowns (degrees of freedom) of the coupled discrete problem. Among the theoretical contributions are the condition number estimates of the BURA-based preconditioners for both positive and negative fractional powers. Ultimately, the analysis of the behavior of the relative condition numbers is aimed at deriving some practical recommendations for minimal BURA orders for the Darcy–Stokes and 3D–1D examples of coupled problems as well as for the related novel approach of non-overlapping domain decomposition preconditioning of elliptic problems.

Variable Neighborhood Search in Hamming space

S.B. Hengeveld, A. Mucherino

The Variable Neighborhood Search (VNS) is one of the most famous and effective meta-heuristic search for global optimization. Proposed by Hansen and Mladenović in 1997, it has been largely employed since then: the article that introduces the VNS has been cited, to date, more than 5000 times.
Although the VNS has already been used for the solution of combinatorial problems, we found that no VNS-based algorithm was specifically designed for performing the search in a Hamming space. Our contribution is an attempt to fill this gap in the long list of VNS variants.
Solution neighborhoods admit very special properties in Hamming space. In continuous space, one can imagine to define bigger neighborhoods when larger distances from the current solution are taken into consideration. In Hamming space, this growth tendency is reversed at a certain point, so that fewer and fewer solutions are actually contained in the neighborhoods related to Hamming distances that are greater than a certain threshold value. At the upper limit, the number of solutions having Hamming distance equal to n from the current solution, where n is the number of bits necessary for the representation of solutions, is 1.
Our implementation exploits these special features implied by the Hamming space for efficiently solving combinatorial optimization problems. Several known VNS variants are taken into consideration and combined with our new neighboring update and search methods in an attempt to find the VNS implementation in Hamming space that is capable to provide the best results. To this aim, we generate instance sets for some known classical problems in combinatorial optimization, such as the Knapsack and Set Cover problems, and we perform an extensive computational comparison of the algorithmic performances.
We implemented all our VNS-based algorithms in Java, and the source codes are all available on the public GitHub's repository named "binMeta".

Randomized Symplectic Model Order Reduction for Hamiltonian Systems

R. Herkert, P. Buchfink, B. Haasdonk, J. Rettberg, J. Fehr

Simulations of large scale dynamical systems in multi-query or real-time contexts require efficient surrogate modelling techniques, such as model order reduction (MOR). One current trend in MOR is the symplectic model order reduction of Hamiltonian systems. A Hamiltonian system has a certain structure which ensures conservation of energy and, under mild assumptions,

stability properties. Classical MOR like the Proper Orthogonal Decomposition (POD) fails to preserve this Hamiltonian structure which, in general, violates the conservation of energy and may yield unstable reduced models. Recently, structure-preserving methods like the complex singular value decomposition (complex SVD) or the SVD-like decomposition have been developed.
In this context, low-rank matrix approximations of the snapshot matrix, such as the truncated singular value decomposition (SVD) are commonly used during the basis computation. In many cases, a randomized approach beats its classical competitor in terms of speed and/or robustness. Here, we show, how the concepts of structure-preserving symplectic basis generation and efficient randomized basis generation can be combined. We present two randomized, symplectic basis generation schemes: a randomized complex SVD (rcSVD) algorithm and a randomized SVD-like (rSVD-like) decomposition. For the rcSVD, we leverage randomization for complex matrices. The rSVD-like algorithm is obtained by a randomized version of the Schur decomposition. We demonstrate the efficiency of the approaches by numerical testing on high-dimensional systems as obtained from spatial discretization of the wave equation.

In Silico Perspective on the Possible Biological Role of the Non-Cationic Peptides in Biologically Active Substances

N. Ilieva, P. Petkov, E. Lilkova, L. Litov

Antimicrobial peptides (AMPs) are a versatile group of small proteins below 10kDa of weight, key elements of the first line of defense against microbial invasion in all classes of living organisms. With the growing bacterial multi-resistance against traditional antibiotics and the very limited resistance developed against AMPs in view, these small molecules appear as promising therapeutic alternative and attract substantial research interest.
The antibacterial activity of AMPs is mainly associated with their cationic and amphiphilic nature, making them electrostatically attracted to the negatively charged bacterial membranes. On the other hand, there is a number of anionic peptides with confirmed antimicrobial action. Moreover, as the AMPs come in nature as part of complex multicomponent substances, the presence there of anionic, cationic and also neutral components has to be investigated in the context of biological activity of the respective substance.
We present *in silico* perspective on the possible modes of action and biological role of non-cationic peptides on the example of newly isolated peptides from the lightest fraction of the mucus of the garden snail *Helix aspersa*. Based on large-scale molecular-dynamics and metadynamics simulations, we study the peptide-membrane-interaction energetics and put forward a hypothesis about the important role of the neutral peptides in the mucus fraction as a transport and local-concentration enhancement system for the biologically active components in the mix.

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Influence of the Grid Resolutions on the Computer Simulated Air Quality Indices Over the Territory of Bulgaria

V. Ivanov, G. Gadzhev, I. Georgieva, K. Ganev, N. Miloshev

The grid resolution would affect the pollution concentrations and thus on the Air Quality Indices (AQI) – a generalized assessment of the air quality impact on human health. Therefore, we made a numerical experiment for evaluation of the horizontal grid resolution impact on the simulated AQI over the territory of Bulgaria. We use a set of models used worldwide – WRF - the meteorological preprocessor, CMAQ - chemical transport model, SMOKE - emission model for performing computer simulations. The "NCEP Global Analysis Data" with a horizontal resolution of 1° x 1° are used as a background meteorological data used in the study. Using the "nesting" capabilities of the WRF and CMAQ models, a resolution of 9 km was achieved for the territory of Bulgaria, by sequentially solving the task in several consecutive, nested areas. Three cases are considered in this paper: Case 1: The computer simulations results from the domain with a horizontal resolution (both of the emission source description and the grid) of 27 km; Case 2: The computer simulations results from the domain with a horizontal resolution (both of the emission source description and the grid) of 9 km; Case 3: Hybrid case with the computer simulations performed with a grid resolution of 9 km, but with emissions like in the 27×27 km domain. The simulations were performed, for all cases and for the period 2008 – 2014, creating an ensemble large and comprehensive enough, reflects the most typical atmospheric conditions with their typical recurrence. The spatial/temporal distribution of the the recurrence of the different AQI categories for Bulgaria are calculated. Comparing them for the above 3 cases makes it possible to evaluate the grid resolution impact.

A Flexible Neural Network Multigrid Solver for the Navier-Stokes Equations

R. Jendersie, N. Margenberg, C. Lessig, T. Richter

We demonstrate the Deep Neural Network Multigrid Solver (DNN-MG) for the incompressible Navier-Stokes equations, a method for machine learning enhanced simulations which improves computational efficiency. A geometric multigrid solver is used in DNN-MG for the coarse levels while a neural network corrects interpolated solutions on fine levels, resulting in a high fidelity solution at significantly lower computational costs. The neural network operates only on small patches of the mesh domain. This local approach greatly facilitates generalizability and allows us to use a network on mesh domains not seen during training. The locality also results in a compact neural network with a small number of parameters, which leads to fast training with limited example simulations and allows for fast evaluation of the network.

In this talk, we discuss the application of Transformers in DNN-MG with a local neighborhood of mesh patches as input, including patches from previous time-steps. Transformers can naturally operate on unstructured meshes and can therefore leverage this context to improve the quality of the prediction. We demonstrate the ability of DNN-MG to generalize to different geometries by training on different flow scenarios.

Some Applications of Compact-Equivalent Operator Preconditioning

J. Karátson

Equivalent operator preconditioning is an organized way to achieve robust, i.e. mesh independent, convergence rates for the iterative solution of various discretized elliptic problems. Mesh independence implies that one may preserve the optimality of a solver of the auxiliary problems regarding the order of operations. This talk considers superlinear convergence based on compact-equivalent operators, whose concept and applications were elaborated in joint work with Owe Axelsson. First some theoretical background is given on preconditioning operators for Krylov iterations, then different applications are shown. The results include robust superlinear convergence for some non-coercive complex problems in Hilbert space, applied to constant and variable coefficient Helmholtz equations, further, streamline diffusion preconditioning for convection-diffusion problems is studied in this context; in addition, the rate of superlinear convergence is analyzed in relation to the integrability of the linearized reaction coefficient.

Adaptive Localized Reduced Basis Methods for Large Scale Parameterized Systems

T. Keil, M. Ohlberger, S. Rave, F. Schindler

For parameterized partial differential equations, the reduced basis (RB) method is a model order reduction (MOR) method allowing for an efficient and certified approximation of the solution manifold. Admittedly, the offline phase for constructing a sufficiently accurate surrogate model can be prohibitively large for problems with a slow convergence of the Kolmogorov n-width, e.g., with a high-dimensional parameter space. On the other hand, spatially global solution methods may easily exceed computational resources in large- or multiscale applications if standard approximation methods are employed for the underlying forward problem.
To remedy both issues, we discuss more recent approaches that go beyond the classical offline-online splitting of MOR methods and adaptively build a surrogate model along a specific quantity of interest. Additionally, we focus on approaches based on a localized reduced basis multiscale method that only requires local solutions but still inherits a global approximation quality due to a respective localized error control.
As a famous use case for adaptive (localized) surrogate models, we show an application to PDE-constrained optimization problems, where an error-aware trust-region method allows for localizing the reduction with respect to the parameter space and enables a certified optimization method with a high convergence rate.

1D-3D Mixed-Dimensional Models Of Tubular Networks Embedded In Porous Media

T. Koch

There are many natural porous media with low permeability. Embedded network systems provide a way to enhance the transport of mass and energy into and from these porous media. Examples of tubular network systems include the blood vessel network in vascularized tissues, plant root systems in soil, networks of petroleum wells, or heat exchangers.
Because the network tube segments are *numerous* (e.g. 10^6) and *thin* in comparison with the model domain, mathematical models for flow and transport processes (including exchange processes between the network and the porous medium) need to be developed with care and constructing efficient numerical methods is a challenge, particularly, methods allowing an accurate approximation of network-bulk exchange processes in combination with reduced model concepts.
We present several recently developed techniques for deriving and solving 1D-3D mixed-dimensional PDE problems. We discuss similarities and differences in the model assumptions. Errors involved with the modeling assumptions are briefly discussed. We show a comparison of methods in numerical test cases and outline numerical challenges. All cases are motivated by relevant applications (tracer transport in biological tissue, root water uptake, well modeling in reservoir engineering).
Finally, for a method based on local mollification combined with local corrections of network-bulk-interface quantities by approximate analytical solutions, we outline how the method can be extended for some nonlinear and anisotropic problems.

Numerical Determination of Source from Point Observation in a Time-Fractional Boundary-Value Problem on Disjoint Intervals

M. N. Koleva, L. G. Vulkov

In the present work, we solve numerically an inverse problem for identification of sources from point observations in a time-fractional diffusion-reaction problem defined on disjoint intervals. The fractional derivative is in Caputo sense with different fractional order on each of the subintervals. We propose algorithms, based on decomposition with respect to the sources on time adaptive mesh. Numerical tests illustrate the efficiency of the proposed approach.

Numerical Determination of Time-dependent Volatility for American Option when the Optimal Exercise Boundary is Known

M.N. Koleva, L.G. Vulkov

We consider the American put option problem for the Black-Sholes equation, which consists in determining of a function $P(S,t)$ for $(S,t) \in [0,+\infty) \times [0,T]$ where t is time, S the underlying asset price, and P is the option price. The definition domain of P is subdivided by an a

priori unknown internal boundary $[s(t),\ t \in [0,T]$ into two parts $\Omega_1 = \{(S,t) : S \geq s(t)\}$ and $\Omega_2 = \{(S,t) : S < s(t)\}$. Here Ω_1 is the contamination region, Ω_2 is the *stopping region*, and $s(t)$ is the *optimal exercise boundary* that must be determined simultaneously with $P(S,t)$. In Ω_1, the function $P(S,t)$ is a solution to the Black-Scholes equation with terminal and boundary conditions.
The position of the internal boundary $s(t)$ at time $t = T$ is $s(T) = K$, where K is the strike price and at other times is determined by the equalities

$$P(s(t),t) = K - s(t), \qquad \frac{\partial P}{\partial S}(s(t),t) = -1 \ \ \forall\, t \in [0,T).$$

After a few changes of independent variables and solution, we arrive at the problem on the region $(y,\tau) \in (0,\infty) \times (0,T)$

$$\frac{\partial p}{\partial \tau} - \frac{1}{2}\sigma^2(\tau)\frac{\partial^2 p}{\partial y^2} - (r(\tau) - d(y,\tau) - \frac{1}{2}\sigma^2(\tau) + \widetilde{s}'(\tau))\frac{\partial p}{\partial y} + r(\tau)p = 0,$$

for the unknown $P(S,t) = p(y,\tau)$ with initial and boundary conditions

$$p(y,0) = 0, \ \ y \in (0,+\infty), \quad \lim_{y\to+\infty} p(y,\tau) = 0,$$

On the boundary $y = 0$, we get two conditions

$$p(0,\tau) = K - \widetilde{s}(\tau), \quad \frac{\partial p}{\partial y}(0,\tau) = -\widetilde{s}(\tau), \ \ t \in [0,T].$$

For the *direct* American put option problem we have to to determine the functions $p(y,t)$ and $\widetilde{s}(t)$. However, if $\widetilde{s}(t)$ is known it is possible one or more of the coefficients of the equation to be identified. Here we determine the volatility $\sigma^2(t)$ numerically, using a decomposition method.

Grid Search Optimization of Novel SNN-ESN Classifier on a Supercomputer Platform

P. Koprinkova-Hristova, N. Kasabov, S. Nedelcheva, S. Ivanovska, S. Yordanov, D. Penkov

This work is demonstrating the use of a supercomputer platform to optimise hyper-parameters of a proposed by the team novel SNN-ESN computational model, that combines a brain template of spiking neurons in a spiking neural network (SNN) for feature extraction and an Echo State Network (ESN) for dynamic data series classification. A case study problem and data are used to illustrate the functionalities of the SNN-ESN. It is a classification problem of EEG data from 14 brain regions that belong to 3 classes related to subjects' movement intention. In one implementation, the SNN consists of 1471 neurons positioned in 3D space according to the Talairach brain template. Neurons are connected via plastic synapses, which strengths are subject to learning using spike-time depending plasticity (STDP) learning rule. The EEG signals are fed into the designed in this way "brain cube" as generating currents into neurons corresponding to the electrodes' positions. The extracted features are the time varying firing rates of all neurons in the cube. Thus, the EEG time series are transformed into spiking activity trends of the representative positions in the brain. An ESN - a fast trainable recurrent neural

network, is then trained to predict the class of the brain activity based on the SNN extracted features. The overall SNN-ESN classifier has several hyper-parameters that are subject to refinement, such as: spiking threshold, duration of the refractory period and STDP learning rate for the SNN part; reservoir size, spectral radius of the connectivity matrix and leaking rate for the ESN part. In order to find the optimal hyper-parameter values exhaustive search over all possible combinations within reasonable intervals was performed using supercomputer Avitohol. The resulted optimal parameters led to improved classification accuracy. This work demonstrates the importance of model parameter optimisation using a supercomputer platform, which improves the usability of the proposed SNN-ESN for real-time applications on complex spatio-temporal data.

Mathematical and Computational Modeling of a Nonlinear Heat Conduction

S. Korotov, M. Křížek

We introduce our main results on solving a nonlinear steady-state heat conduction problem of nonmonotone type in anisotropic and nonhomoge- neous media and its finite element approximation. In particular, we con- centrate on temperature distribution typical for e.g. large transformers and rotary machines. We present theorems on the existence and uniqueness of weak and discrete solutions and their convergence. For example, if the heat conduction coefficients are Hölder continuous, the weak solution exists and is unique. On the other hand, for continuous (but not Hölder continuous) ones we may get infinitely many weak solutions for given boundary conditions. We also mention how to treat numerically a nonlinear radiation boundary condition.

Exploring the Global Solution Space of a Simple Schrödinger-Poisson Problem

R. Kosik, J. Cervenka, D. Waldhör, F. Ribeiro, H. Kosina

Quantum electron transport in nanostructures can be described by a coupled Schrödinger-Poisson system. For the simulation of IV-characteristics we need to solve the stationary system self-consistently with the bias as a varying parameter, which presents a continuation problem. For the solution of the nonlinear system we use bias-stepping combined with a full Newton method. The k-grid representing the injected Schrödinger modes is refined adaptively. Parallelization is employed for the assembly of the Jacobian.
In general the solution to a nonlinear system need not be unique. We monitor the number of negative eigenvalues in the Jacobian in order to detect path switching when bias-stepping.
For bulk we find two self-consistent solutions at each bias point with zero and one negative eigenvalue in the Jacobian respectively. We then simulate simple nin-structures (doping well). For an exemplary nin-structure, bias-stepping upwards starting from equilibrium runs into a bifurcation point. From the bifurcation point emerges a second solution path stepping downwards in the bias.

The selected simulation examples demonstrate numerically that the solution to the Schrödinger-Poisson model at a fixed bias is in general not unique and the global solution structure of the continuation problem is non-trivial.

Non-overlapping DD-BURA preconditioning for 3D elliptic problems

N. Kosturski, S. Margenov, Y. Vutov

Let us consider the Poisson equation $-\Delta u = f$ in the polyhedral domain $\Omega \subset \mathbb{R}^3$, equipped with appropriate boundary conditions on $\Gamma = \partial\Omega$. Assume that the finite element method (FEM) is applied for numerical solution of the problem using linear elements on a quasi-uniform tetrahedral mesh $\mathcal{T}_h$, thus obtaining the linear system $A\mathbf{u} = \mathbf{f}$. Now let $\{\Omega_i\}_{i=1}^m$ be a non-overlapping partitioning of Ω with interface γ. We do not suppose any special restrictions on the geometry of the 2D manifold γ. The stiffness matrix A is written in the form

$$A = \begin{pmatrix} A_D & A_{D\gamma} \\ A_{\gamma D} & A_\gamma \end{pmatrix},$$

where the blocks A_i correspond to the subdomains Ω_i, $i = 1, 2, \cdots, m$, and A_γ - to the interface. We study the following multiplicative non-overlapping domain decomposition (DD) preconditioner

$$C_{DD,k}^{BURA} = \begin{pmatrix} A_D & \\ A_{\gamma D} & \sigma C_{1/2,k}^{BURA}(\Lambda) \end{pmatrix} \begin{pmatrix} I & A_D^{-1} A_{D\gamma} \\ & I \end{pmatrix}.$$

The parameter $\sigma > 0$ does not depend on the mesh size h. The block $C_{1/2,k}^{BURA}(\Lambda)$ is implicitly defined. Its inverse is the best uniform rational approximation (BURA) of degree k of $\Lambda^{-1/2}$, where Λ is the discrete Laplacian corresponding to $\mathcal{T}_h \cap \gamma$. The main theoretical result is that $C_{DD,k}^{BURA}$ is an asymptotically optimal preconditioner, i.e. it's computational complexity is $O(N)$. Our analysis shows that relatively small degree k is enough to stabilize the number of PCG iterations. On the other hand, it is worth noting that the degree k has a decreasing effect on the overall computational complexity as the problem size N increases. The large-scale numerical tests performed confirm the computational efficiency and robustness of the presented next-generation non-overlapping domain decomposition approach for 3D elliptic problems.

High-Order Small-Time Local Controllability

M. I. Krastanov, M. N. Nikolova

A class of polynomial control systems with bounded controls is considered. The local properties of the corresponding reachable sets are studied by using the Campbell-Baker-Hausdorff formula. The main result is a sufficient condition for small-time local controllability. Two four-dimensional examples illustrate the applicability of the proposed approach.

On the Euler Equation

M. Krastanov, N. Ribarska

The basic problem of calculus of variations with locally Lipschitz criterion is considered in the presence of pure state constraints of equality type. A necessary optimality condition is obtained under suitable assumptions. An example illustrating the applicability of the obtained results is presented.

A Sufficient Condition for the Existence of a Nash Equilibrium

M. I. Krastanov, B. K. Stefanov

A discrete dynamical game is considered on an infinite-time horizon. A sufficient condition for the existence of a Nash equilibrium is proved under suitable assumptions. An illustrative example shows the applicability of the proposed approach.

Breaking the Curse of Dimensionality with Active Subspaces

S. Kucherenko, O. Zaccheus, O. Zaccheus

High dimensional problems pose a significant challenge due to the curse of dimensionality. It concerns machine learning, global optimization, uncertainty quantification and other applications. Such problems benefit tremendously from proper dimension reduction. One way to break the curse of dimensionality is to identify and exploit special structure in the model. Active subspaces (AS) is a method which identifies important directions in the parameter space and allows significant dimension reduction. Consider a nonlinear numerical model $f(x) \in L_1$, where $x \in R^n$ is distributed according to a pdf $p(x)$. Compute the symmetric positive semidefinite matrix $C = E[\nabla f \nabla f^T]$ and its eigenvalue decomposition: $C = W \Lambda W^T$, where $\Lambda = diag(\lambda_1, ..., \lambda_n), \lambda_1 \geq ... \geq \lambda_n$ are eigenvalues and W is the orthogonal matrix of the corresponding eigenvectors forming the basis of R^n. The main idea of the AS method is to find a partition $W = W_1 + W_2$, where W_1 is formed by the eigenvectors of the top k eigenvalues (where $k \ll n$), such that $f(x) \approx g(x)$, where $y = W_1^T x, y \in R^k$ is called an active variable. The span of the top k eigenvectors of C is called the "active" subspace. It can be shown that optimal (in a certain sense) k corresponds to the largest gap in the spectrum of C. Notice that unlike the global sensitivity analysis techniques which find the most important design variables (directions aligned with the axes of the parameter space), the AS method provides a linear combination of all design variables that mostly affects the output (directions typically not aligned with the axes of the parameter space). Perturbing the inputs along the important directions causes greater change in the prediction, on average, than perturbing along the unimportant ones. The straightforward way to exploit the active subspace is to build a surrogate model $g(y)$ in the low dimensional space of active variables. We developed a framework which allows to effectively build surrogate models which then are used to 1) compute Sobol' sensitivity indices and other global sensitivity measures; 2) solve surrogate-based optimization problems; 3) find critical model regions. The last point is related in particular to identification of the design

space, namely finding the ranges of parameters that guarantee required specifications of the output.

Domain Decomposition Solvers for Problems with Strong Fractional Interface Perturbations

M. Kuchta

Operators consisting of an elliptic part in the bulk domain and a parameter-weighted interface perturbation of fractional order arise in the context of preconditioning of coupled multiphysics systems, e.g. in formulations of Stokes-Darcy or Stokes-Biot problems, where the coupling is enforced without Lagrange multipliers. Parameter-robust approximation of the inverse of such operators presents a challenge for standard black-box algorithms. In this talk we develop robust and scalable solvers for interface-perturbed operators based on domain/subspace decomposition. In particular, we discuss posing of an auxiliary interface problem in the intersection space of weighted fractional order Sobolev spaces and show that the corresponding Riesz map can be efficiently realized by rational approximations. Performance of the developed solvers will be demonstrated on single and multiphysics examples.

Earth Observation Data Processing Simulator Based on the CloudSim

A. Lalayan, H. Astsatryan, G. Giuliani

Earth observation (EO) data contains various important information for the different cases of environmental monitoring at the local and global scale. The Big EO data processing workflows require High-Performance Computational (HPC) resources to parallelize the tasks across multiple processors in parallel computing environments. EO communities widely use the Dask parallel python framework to improve data processing performance via partitioning the data by chunk size across Dask workers. The community strives to determine for EO workflows the best trade-off between costs and performance depending on the composition, configuration, and deployment of the Dask clusters, such as the number and computational characteristics (CPU, RAM, etc.) of Dask clusters. It is required to carry out a lot of experiments or to use modelling and simulation tools to increase the accuracy of resource provisioning by considering a wide range of parameters to choose optimal Dask cluster configurations satisfying the EO workflow needs. How- ever, the experiments under varying load, performance, or system size are costly, while the simulation tools support generalized applications. To overcome this challenge, a user-friendly simulator tool based on the CloudSim simulator is proposed for EO data processing workflows. The tool reduces the average resource utilization of the Dask clusters and energy consumption by applying it in decision-making systems. The evaluation results show high accuracy between the actual experiments and the tool results.

Robust Preconditioned Iterative Solvers for Discretized Reduced Optimality Systems

U. Langer, R. Löscher, O. Steinbach, H. Yang

We propose, analyze, and test new robust iterative solvers for systems of linear algebraic equations arising from the finite element discretization of reduced optimality systems. We consider optimality systems defining the optimal state y, adjoint p, and control u of elliptic, parabolic, and hyperbolic distributed optimal control problems with both the standard L_2 and the more general energy regularizations.

In contrast to the usual time-stepping approach, we discretize the optimality system arising from time-dependent optimal control problems by space-time continuous piecewise-linear finite element methods on fully unstructured simplicial meshes in the same fashion as in the case of elliptic problems. After eliminating the control u from the optimality system, we arrive at the reduced optimality system that, after its (space-time) finite element discretization, turns into one large-scale, but sparse, symmetric, indefinite, and regular algebraic system for defining the finite element approximations y_h and p_h to y and p, where h stands for the usual mesh size parameter. We can further reduce this system to a symmetric and positive definite Schur complement system by eliminating p_h.

If we aim at the best approximation of the given desired state y_d by the computed finite element state y_h, then the optimal choice of the regularization parameter ϱ is h^4 and h^2 for the L_2 and the energy regularization, respectively. The convergence rate is the same as the best approximation rate that only depends on the regularity of y_d. It turns out that, for this choices of ϱ, the mass matrix and, therefore, suitable simple diagonal approximations of it deliver spectrally equivalent preconditioners for the Schur complement matrix. This result can rigorously be proven, at least, for the L_2 regularization. On the basis of this observation, we can construct robust (parallel) iterative solvers for the reduced finite element optimality systems. These results can be generalized to variable regularization parameters adapted to the local behavior of the mesh-size that can heavily change in case of adaptive mesh refinement. The numerical results confirm the theoretical findings.

On Scalability of Hybrid Monte Carlo Methods on Advanced Architectures and their Sensitivity to True Random Numbers

A. Lebedev, E. Sahin, V. Alexandrov

This paper provides the results of our current investigation of the applicability of hybrid Monte Carlo methods for solving systems of linear algebraic equations to a variety of problems in science and engineering. Markov Chain Monte Carlo Matrix Inversion (MCMCMI) is our method of choice and we investigate its use as a preconditioner in combination with GMRES and (Bi) CG(stab) methods to solve a variety of problems arising in quantum chromodynamics, plasma physics and engineering. Representative matrices for the latter two are extracted from BOUT++ and Nektar++ implementations of specific simulation scenarios. We present our results on the performance and scalability of the implementations of the method in C++/CUDA and Python/CuPy for a variety of CPU and GPU architectures (e.g., P100, V100, A100) as well as our observations on the effects of using true random number generators (TRNGs).

Unravelling the Mechanism of Action of the SARS-CoV-2 ORF6 Protein Using Computer Simulations

E. Lilkova, P. Petkov, M. Rangelov, N. Todorova, L. Litov, N. Ilieva

Open reading frame 6 (ORF6) is an accessory protein, uniquely expressed in the virus subgenus, to which SARS-CoV and SARS-Cov-2 belong. Its primary function is to suppress the host innate immune antiviral response by antagonizing with type-I interferon signaling. In addition, ORF6 is the most toxic protein of the virus and contributes significantly to COVID-19 lung pathology and disease outcome, which prompts active search for possible inhibitors of this protein. However, despite the significant research focus and efforts, ORF6 is one of the dozen proteins of SARS-CoV-2, whose 3D structures have not yet been resolved, hindering substentially the development of inhibitors.
The SARS-CoV-2 ORF6 is a small protein, containing 61 amino acid residues. It targets the Rae1-Nup98 complex, which contributes to mRNA nuclear export. ORF6 is a membrane protein but contains a highly acidic flexible solvent-exposed C-terminal tail. This part of the protein is considered responsible for its interaction with the cellular Rae1-Nup98 complex.
Here, we report the development of a structural 3D model of the SARS-CoV-2 ORF6, embedded in a model endoplasmic reticulum membrane. Then, the interaction of ORF6 and RAE1 is explored using long-scale molecular dynamics simulations. We demonstrate that the proteins bind via the flexible C-terminus of ORF6 and form a stable complex. Some preliminary results on the search for suitable potential inhibitors of the protein are also discussed.

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Compensated Multifold Preconditioners

H. Lu, C. Blom, J. Vink

This paper describes compensated multifold preconditioners including the concepts, framework and algorithms. Firstly, a manifold preconditioner framework is designed to deal with a variety of preconditioners in a uniform way. The framework can be used to implement most preconditioning methods, for example, algebraic multigrid, (block) incomplete factorization, domain decomposition, Schur complement preconditioning and so on. Secondly, multifold structures are introduced to reorganize data used for preconditioner construction using two dimensional recursive relations. Thirdly, a compensated multifold preconditioner is constructed for a large sparse (block) matrix by applying the manifold preconditioner framework and the two dimensional recursive relations of the mutifold structure. The following concepts and algorithms are used in each recursion:

- Recursive computation of an approximate inverse of a compensated multifold preconditioner.

- Product rules in approximating the Schur complement to control the sparsity of the approximate Schur complement.
- Block diagonal compensation to compensate the approximate Schur complement.
- Sparsity control to control the sparsity of the compensated multifold preconditioner to prevent fillins blown out.

An algorithm of solving compensated multifold preconditioner systems is introduced as well using two dimensional recursive relations. Finally, the compensated multifold preconditioner is applied in real reservoir simulation. Running with several assets shows that the compensated multifold preconditioner reduces the number of linear iterations by 1.5 to 4 times depending on the size of timestep in comparison with the preconditioner BILU(k) popularly used in reservoir simulation. The larger the timestep, the bigger the reduction of linear iterations. Consequently, the compensated multifold preconditioner considerablely improves the performance of whole simulation.

Economic Implementation of the ORBD Preconditioning for Discretized Optimal Control Problems Constrained With Fractional Diffusion Equations

K.-Y. Lu

For a class of optimal control problems constrained with certain time- and space-fractional diffusion equations, by making use of mixed discretizations of temporal finite-difference and spatial finite-element schemes along with Lagrange multiplier approach, we obtain specially structured block two-by-two linear systems. Then we construct a rotated block-diagonal preconditioning matrix, analyze spectral properties of the corresponding preconditioned matrix, and present an economic implementation of the approximated rotated block-diagonal preconditioner. Both theoretical analysis and numerical experiments show that the preconditioned Krylov subspace iteration methods, when incorporated with these rotated block-diagonal preconditioners, can exhibit optimal convergence property in the sense that their convergence rates are independent of both discretization stepsizes and problem parameters, and their computational workloads are linearly proportional with the number of discrete unknowns.

Numerical Comparison of Block Preconditioners for Poroelasticity

T. Luber, S. Sysala

Poroelastic models describe a coupled solid-fluid interaction. We consider Biot's model that describes the deformation of the solid skeleton by linear elasticity and the fluid flow by Darcy's law. The focus of the talk is on the formulation in displacements, fluid flux and fluid pressure after the discretization in time by implicit Euler method. This leads to a linear system with a natural 3×3 block structure.

Preconditioner based on the Schur complement with respect to pressure will be presented and analysed and compared with several block preconditioners that arise from algebraic and functional constructions. The preconditioners will be used in preconditioned Krylov methods and compared in the terms of numbers of iterations. For the numerical experiments, we will focus on geotechnical settings and test the dependence of performance of individual preconditioners on the parameters of the model.

On Locally Uniformly Rotund Renorming of the Space of Continuous Functions on a Compact Admitting a Fully Closed Projection

T. Manev, S. Troyanski

We show that if the compact space X admits a fully closed projection onto a compact Y such that $C(Y)$ admits an equivalent locally uniformly rotund (LUR) norm, as do the spaces $C(\pi^{-1}(y))$ for all y in Y, then $C(X)$ is also LUR renormable. A continuous map $\pi : X \to Y$ between Hausdorff compacta is called fully closed if the intersection $\pi(A) \cap \pi(B)$ is finite whenever A and B are closed disjoint subsets of X. As a main corollary, we prove that $C(K)$ admits an equivalent LUR norm if K is a Fedorchuk compact of finite spectral height.

The Tensor-Train Mimetic Finite Difference Method For Three-Dimensional Maxwell's Wave Propagation Equations

G. Manzini, D. M. P. Truong, R. Vuchkov, B. Alexandrov

Coupling the mimetic finite difference method with the tensor-train format results in a very effective method for low-rank numerical approximations of the solutions of the time-dependent Maxwell wave propagation equations in three dimensions. In such numerical algorithm, we discretize the curl operators on the primal/dual tensor product grid complex and we couple the space discretization with a staggered-in-time second-order accurate time-marching scheme. The resulting solver is compatible and accurate to the second order in time and space, and the approximation of the magnetic flux field has zero discrete divergence. Employing the tensor-train format improves the solver performance by orders of magnitude in terms of CPU time and memory storage. A final set of numerical experiments confirms this expectation. .

Multiagent Systems, Nonlinear Superposition and Random Lift

A. Marigonda

Multi-agent systems are systems where the number of possibly interacting agents is so large that only a statistical description is viable. Such kind of systems can be viewed as a sort of

nonlinear superposition of underlying finite-dimensional systems, where nonlinearity arises in consequence of the mutual interactions of the agent.
One of the most challenging problem in this framework is given by the study of properties of the underlying finite-dimensional systems that are preserved in the superposition system.
In this talk we will present some recent results concerning tools used to study optimization problems in the setting of multi-agent systems, obtained in collaboration with Rossana Capuani (University of Tuscia).

Two Approaches for Identifying COVID-19 Parameters Illustrated with Data for Bulgaria

T. T. Marinov, R. S. Marinova

This work is focused on special numerical techniques for identifying time-dependent epidemics parameters such as transmission and removal rates, and the corresponding basic and effective reproduction numbers.
The first method is based on solving the inverse problem for coefficients' identification in an Adaptive Susceptible-Infected-Removed (A-SIR) epidemic model with time-dependent transmission and removal rates.
The second approach is based on a partial integral of the SIR system of ordinary differential equations and the least square method. It is limited to estimation of the basic and effective reproduction numbers.
The developed methods are used for identifying the parameters with real data for COVID-19 reported for Bulgaria. The results demonstrate how well the methods simulate the dynamics of the infectious disease.

A Functional Tensor Train Library in RUST for Numerical Integration and Resolution of Partial Differential Equations

M. Martinelli, G. Manzini

Low-rank tensor decomposition schemes were originally developed to construct approximations of high-dimensional tensors. Within the last decade, Tensor-Train decomposition, a form of tensor decomposition that does not inherently suffer from the curse of dimensionality, gained a lot of popularity due to its mathematical properties.
In the last few years the continuous generalization of Tensor-Train decomposition, called Function-Train decomposition, was introduced. This decomposition allows to approximate high-dimensional functions without the needs of function sampling and allowing a flexible framework for function integration and differentiation.
In this talk we present a new library written in RUST that is aimed to provide functionalities for Function-Train decomposition. The library also provides methods for continuous matrix factorizations and continuous multilinear algebra operations, like addition, multiplication, integration, differentiation, etc.
Examples of application of the library for numerical integration and resolution of PDEs will be also presented.

The Modeling Error in Reduced 3D-1D Time Dependent Solute Transport Models

R. Masri, M. Zeinhofer, M. Kuchta, M. E. Rognes

Topologically reduced 3D-1D models of solute transport provide a computationally efficient alternative to fully coupled 3D-3D models. Such reduced models are suitable for simulations in large 1D vessel networks embedded in 3D tissue. We estimate the error introduced between the reduced model and a corresponding reference 3D-3D model in evolving domains. Such apriori estimates are derived in suitable Bochner spaces via duality arguments. Further, we analyze the discretization error of the reduced problem which poses interesting challenges due to the lack of full H^2 regularity. Numerical results confirm our theoretical findings.

A Variational Mean Field Game with Free Final Time and Control Interaction

G. Mazanti, L. Pfeiffer, S. S. Arjmand

In this talk, we present a mean field game model with control interaction in which an agent's optimization criterion consists in minimizing a certain cost in free final time with the constraint of reaching a given target set. More precisely, the cost of an agent is made of an individual running cost, a pairwise interaction cost which takes into account both positions and velocities of the agents, and a cost on the time the agent takes to reach the given target set, which is equal to $+\infty$ if the target set is not reached.
After presenting the framework, its motivation from the modeling of crowd motion, and some previous related results for minimal-time mean field games and other similar mean field game models, we present our main result, which provides a potential structure for the game by showing that its equilibria can be characterized as critical points of a functional $\mathcal{J}$. This is done by adopting a Lagrangian description of the game, and existence of equilibria is obtained after studying the existence of a minimizer of $\mathcal{J}$.
We also discuss the numerical approximation of equilibria for the corresponding N-player game. Thanks to the potential structure of the N-player game, we make use of a best response dynamics, which can be interpreted as a coordinate descent algorithm on the functional $\mathcal{J}$. The talk is concluded by numerical illustrations.

Algebra Preconditionings for 2D Riesz Distributed-Order Space-Fractional Diffusion Equations on Convex Domains

M. Mazza, R. Sormani, S. Serra-Capizzano

When dealing with the discretization of differential equations on non-rectangular domains, a careful treatment of the boundary is mandatory and may result in implementation difficulties and in coefficient matrices without a prescribed structure. Here we examine the numerical

solution of a two-dimensional constant coefficient distributed-order space-fractional diffusion equation with non linear term on a convex domain. To avoid the aforementioned inconvenience, we resort to the volume-penalization method, which consists in embedding the domain into a rectangle and in adding a reaction penalization term to the original equation that dominates in the region outside the original domain and annihilates the solution correspondingly. Thanks to the volume-penalization, methods designed for problems in rectangular domains are available for those in convex domains and by applying an implicit finite difference scheme we obtain coefficient matrices with a 2-level Toeplitz structure plus a diagonal matrix which arises from the penalty term. As a consequence of this, we can describe the asymptotic eigenvalue distribution as the matrix size diverges as well as estimate the intrinsic asymptotic ill-conditioning of the involved matrices. On these bases, we discuss the performances of the conjugate gradient with circulant and τ-preconditioners and conduct related numerical experiments.

Viscous Regularization of the MHD Equations

M. Nazarov

Nonlinear conservation laws such as the system of ideal magnetohydrodynamics (MHD) equations may develop singularities over time. Viscous regularization is a common approach to avoid such situations while obtaining a convergent solution sequence. This talk presents a new viscous flux to regularize the MHD equations. Our proposed viscous flux combines the Guermond-Popov flux [Guermond-Popov, 2014] for compressible flows and the resistivity flux for the magnetic component. We prove that the proposed viscous flux holds attractive properties such as it preserves the positivity of density and internal energy, it satisfies the minimum entropy principle, it is consistent with all the generalized entropies, and it is Galilean and rotationally invariant. The proposed viscous regularization has numerically experimented with an artificial viscosity finite element method. The numerical results show that: (i) high-order accuracy is obtained for smooth solutions; (ii) shocks and other discontinuities are finely captured; (iii) the numerical behaviors are strongly aligned with the continuous analysis; (iv) the proposed viscous flux behaves similarly to the resistive MHD flux in the magnetic reconnection test with physical viscosity.
This is a collaborative work with Tuan Anh Dao and Lukas Lundgren from Uppsala University.

The Power of Block Preconditioners

M. Neytcheva

The presentation surveys some preconditioners for two-by-two block matrices and discusses their properties and mutual relations. Consider matrices

$$\mathcal{A} = \begin{bmatrix} A & B^T \\ B & C \end{bmatrix} \quad \text{or} \quad \mathcal{A} = \begin{bmatrix} A & B^T \\ B & -C \end{bmatrix},$$

where $A \in \mathbb{R}^{n\times n}$, $C \in \mathbb{R}^{m\times m}$, $B \in \mathbb{R}^{m\times n}$, $n \geq m$.

As is well known, the applications where such structured matrices occur, are multifold. These can arise from discrete systems of partial differential equations, the structure can be obtained by using some recursively defined 'fine-coarse' mesh hierarchy or in a fully mesh-independent way, permuting a given matrix in a way, proficient in some particular context, etc.
With the initial assumption that A is nonsingular, as is also well known, using the framework of block-Gauss factorization, $\mathcal{A}$ can be factorized as

$$\mathcal{A} = \mathcal{LDU} = \begin{bmatrix} I_n & 0 \\ BA^{-1} & I_m \end{bmatrix} \begin{bmatrix} A & 0 \\ 0 & S \end{bmatrix} \begin{bmatrix} I_n & A^{-1}B^T \\ 0 & I_m \end{bmatrix}. \tag{1}$$

The major terms in the factorization as well as in the most broadly used preconditioning techniques for matrices with the given structure are the block A and the Schur complement $S = C \mp BA^{-1}B^T$, respectively.
We first recall some existing general results regarding the eigenvalues of the saddle point form of the matrix $\mathcal{A}$, then for its preconditioned form and how approximations of A and S affect the spectrum of these preconditioned systems.
We next consider $n = m$ when, in addition to the classical preconditioners based on the factorization in (1) and using the properties of the blocks, other preconditioners have been defined, one of them being the so-called PRESB preconditioner $\mathcal{P} = \begin{bmatrix} A & -B^T \\ B & A + B + B^T \end{bmatrix}$ for $\mathcal{A}$ of the form $\mathcal{A} = \begin{bmatrix} A & -B^T \\ B & A \end{bmatrix}$, its relations to some of the preconditioners, based on (1) and some variants suited for nonsymmetric and singular blocks.

Tensor Train Approximation and Monte Carlo Methods in High Dimensional Optimal Control Problems

M. Oster

We will display two approaches in order to approximatively solve Bolza type finite horizon Optimal control problems. The first approach is to solve the associated Bellman equation numerically by employing the Policy Iteration algorithm. In a second approach, we will introduce a semiglobal optimal control problem and use open loop methods arising from a Pontryagin maximum principle on a feedback level. To overcome computational infeasability we use low rank hierarchical tensor product approximation/tree-based tensor formats, in particular tensor trains (TT tensors) and multi-polynomials, together with high-dimensional quadrature, e.g. Monte-Carlo. By controlling a destabilized version of viscous Burgers and a diffusion equation with unstable reaction term numerical evidence is given.

Optimization and Sensitivity Analysis of a Parallel Code for Air Pollution Modelling

T. Ostromsky, V. Todorov, K. Georgiev, I. Dimov, Z. Zlatev

The environmental modelling and air pollution modelling in particular is one of the toughest problems of computational mathematics (together with the meteorological modelling). All

relevant physical and chemical processes in the atmosphere should be taken into account, which are mathematically represented by a complex PDE system. To simplify it a proper splitting procedure is applied. As a result the initial system is replaced by several simpler systems (submodels), connected with the main physical and chemical processes. These systems should be calculated in a large spatial domain, as the pollutants are moved quickly by the winds on a long distance, especially in the upper layers of atmosphere. The dynamics of the atmospheric processes require small time-step to be used in order to get a stable numerical solution of the corresponding system. Sensitivity analysis of the model outputs to variation of some parameters or natural uncertainty of the input data is another important issue for improving the reliability of such a model. Sobol approach, based on stochastic multidimensional integration algorithms is applied for that purpose.

These heavy and time-consuming computational tasks have always been a serious challenge, even for the fastest and most powerful supercomputers nowadays. In this talk we present the overtaken challenges and novel results obtained by using the new Bulgarian petascale supercomputer Discoverer.

Numerical Modelling of the Nucleation and Growth of Multiple Three-Dimensional Dense Fracture Sets

A. Paluszny, M. C. Saceanu, R. W. Zimmerman

In this work, a three-dimensional finite element-based technique is used to propagate multiple fractures in a brittle rock unit. This iterative approach models the quasi-static growth of multiple fractures following two events, which translate into two different remote stress scenarios. Each remote stress scenario produces a fracture set containing hundreds of discrete fractures. During the first stage, one set of fractures is grown in response to the remote stresses; thereafter, a second set having differing orientation is generated within the same domain. The rock matrix is assumed to be isotropic and linear elastic. For the two-set generation, two cases are investigated: (a) a spatially uniform Young's modulus and fracture toughness, and (b) a normal distribution of these properties with a prescribed variation. Three criteria form the basis of the growth algorithm: a strain rate-dependent damage-based nucleation criterion, a stress intensity-based multi-modal fracture propagation criterion, and the Richard/Schoellman criterion for the propagation angle. During the simulation, small-scale disk-shaped discontinuities are added to the domain following the nucleation criterion. These discontinuities can grow in response to stresses, and also merge and coalesce in response to stresses. In order to handle fracture arrest, closure, and coalescence geometrically, fracture geometries are tracked independently of the computational mesh that is used to calculate the displacement and stress fields. To account for changes in the displacement field and geometry, the mesh is adaptively re-meshed. The model reproduces en-echelon crack linkage, fracture hooking, and orthogonal tip approximation patterns. Patterns are shown for sequential deformation stages. The density and fracture aperture distribution of the ensuing fracture patterns are quantified. The resulting meshes contain thousands of geomechanically grown fractures, with around 4 million nodes, and around 12 million degrees of freedom. Details of strategies to model large-scale fracture growth systems will also be discussed.

About Methods of Vector Addition over Finite Fields using Extended Vector Registers

M. Pashinska-Gadzheva, I. Bouyukliev

We present optimized algorithm for vector addition over finite prime fields using the extended vector registers of modern central processing units (CPU) and the corresponding extended Intel instruction sets SSE4.1 and AVX2. The presented algorithm is based on representation of the elements of the fields using unsigned 8-bit packed integer, thus allowing for computations over prime fields with up to 127 elements. The efficiency of the presented method is demonstrated in an algorithm for calculating the weight distribution of a linear code over the finite field which is known to be an NP-complete problem. An optimized approach for computing the weight of a vector is also given. The experimental results show faster execution times compared to the corresponding algorithms in the Magma and GAP packages for finite fields larger than 3 (for smaller fields there is natural bitwise representation). For example considering linear codes over GF(17) the proposed algorithm is approximately 6 times faster than Magma and more than 190 times faster than the Guava package for GAP.

Flow Simulations In Large-Scale Fractured Media

G. Pichot

In underground environments, fractures are numerous and present at all scales (from cm to km), with very heterogeneous properties. They are difficult to locate and image accurately either by direct observations of wells or by geophysical prospecting. The most commonly used model for fractured rocks is the Discrete Fracture Matrix (DFM) model, in which fractures are represented as structures of codimension 1 (Discrete Fracture Network - DFN). In this work, stochastic DFNs are generated with the software DFN.lab (`https://fractorylab.org/dfnlab-software/`). It enables the generation of cubic-meter fractured rocks, containing over one million of fractures. To estimate the effects of the uncertainty of the geometry and properties of fractures on the overall flow field, multiple DFN realizations are required and for each of them, a flow simulation is performed. Such an ensemble approach is feasible provided each simulation is quite cheap.
This motivates us to propose and build an efficient methodology for flow simulation in such large-scale fractured rocks. To gain computational time and resources, we propose to combine advanced meshing and discretization techniques, together with robust solvers for the underlying linear systems. The mesh generation of the DFN is performed with the software MODFRAC, developed by Inria (Gamma and Serena teams) and the University of Troyes. The volumic mesh is realized with the Inria software GHS3D (Gamma team). For discretization, we focus on Hybrid High-Order (HHO) methods. HHO produces high-order, optimally converging, and locally conservative discrete solutions. HHO methods are closely related to Hybridizable discontinuous Galerkin methods and support general meshes (polygonal, polyhedral). After static condensation, the globally coupled unknowns are face polynomials of order $k \geq 0$. Combined with a posteriori error estimates and mesh coarsening strategies, such methods reduce the number of unknowns without compromising the accuracy of the numerical solution. To solve the large-scale linear systems, we propose to use HPDDM (`https://github.com/hpddm/hpddm`), the high-performance unified framework for domain decomposition methods. Several benchmark test cases will be presented to illustrate the benefit of the proposed methodology.

Stationary Mean Field Games With State Constraints

A. Porretta, M. Ricciardi

We investigate elliptic mean field game systems in a bounded domain Ω, where the optimal control for the generic player is chosen from the controls with ensures the invariance of the domain Ω. The existence of blowing-up solutions for the Hamilton-Jacobi equation was already studied by J.-M. Lasry and P.-L. Lions, and a precise estimate for the behaviour of the solutions near the boundary was proved by A. Porretta and T. Leonori. Here, we improve these results, obtaining an estimate of D^2u near the boundary. Then we study the Fokker-Planck equation, showing how the estimates on u yield the existence and uniqueness of solutions in L^1. Moreover, we can also prove a global $H^1_0 \cap L^\infty$ estimate on m, which vanishes at the boundary with a rate of d^θ, where $\theta \geq 2$ is related to the Lagrangian of the control problem. This allows us to obtain existence and uniqueness of solutions for the Mean Field Games system.

The Wright Function – Numerical Approximation and Hypergeometric Representation

D. Prodanov

Fractional calculus models of physical phenomena have rekindled the interest in special mathematical functions. The Wright function, which arises in the theory of the space-time fractional diffusion equation, is a very general mathematical object with diverse connections to other special and elementary functions. Notably, it provides a unified treatment of several classes of special functions, such as the Gaussian, Airy, Bessel, error functions, etc. The objective of the present contribution is two-fold. On the first place, the paper presents a numerical integration technique for approximation of the Wright function using using the method of stationary phase. The algorithm uses the double-exponential quadrature integration method. On the second place, the paper exhibits a symbolical algorithm for hypergeometric (HG) representation of the Wright function $W(a, b\,|x)$. For rational values of its first argument the function is reduced to a finite sum of HG functions and polynomials. The HG functions are themselves represented by known elementary or other special functions, wherever possible. Reference implementations of the algorithms are programmed in the open-source computer algebra system Maxima.

Subtransversality and Measures of Noncompactness

N. Ribarska, M. Krastanov

A sufficient condition for tangential transversality involving measures of non-compactness as well as a Lagrange multiplier theorem for the infinite-dimensional optimization problem are obtained. The relation of the obtained results to the basic problem of calculus of variations is discussed. Also, an application to the problem of calculus of variations in the presence of pure state constraints of inequality type is presented.

Transversality and Strong Tangetial Transversality

N. Ribarska, M. Tasheva

The relation between the properties transversality and strong tangential transversality of sets in a Banach space is explored. It is obtained that for two sets in a Banach space strong tangential transversality implies transversality and the reverse implication fails. An application to Banach space theory is presented. A definition of strong tangential transversality for a finite number of sets is proposed which preserves the main properties of the notion.

Integrating Quantum Machine Learning with Computational Histopathology for Cancer Slides Classification

E. Sahin, S. Mensa, P. Pati,
A. F. Rodriguez, J. L. Robertus, M. Gabrani

In this study, we propose the use of Quantum Computing in Computational Pathology (QC-CP) to improve the accuracy of disease diagnosis and treatment selection. By utilizing Quantum Machine Learning (QML) tools, we aim to enhance traditional ML approaches in the field of histopathology. Specifically, using Quantum Kernel methods in Support Vector Machines (SVMs) for image classification, we aim to exploit the high dimensionality of the Quantum Hilbert space to linearly separate data into the right diagnostic classes. The method involves feeding low-resolution cancer slides to a deep neural network to extract embedded features, which are then reduced and encoded into a quantum circuit to produce a quantum kernel. The results show that this method with reduced image definition and number of features can perform just as well as a histopathology domain specific Graph Neural Network (GNN) fed with high-resolution slides, and in some instances can perform more accurate classification of slides. This is an important first step towards the integration of QC with CP, suggesting that QML may provide matching or improved classification results using low-resolution slides, potentially reducing the training time of the model.

Flexible Multigrid Methods within the Finite Element Library NGSolve

J. Schöberl

In this talk we discuss a collection of multigrid based preconditioning methods, and how to use and combine them within the finite element package NGSolve. The performance critical components are implemented in C++, and a Python interface allows a flexible combination on a high level language. Examples are low-order / high-order finite element methods, auxiliary space preconditioning, algebraic multigrid methods, and the utilization of third party highly parallel multigrid libraries. We discuss different goals for teaching, research and application of multigrid methods.

Indifference Thresholds in a Bi-Objective Capital Accumulation Problem

A. Seidl, R. F. Hartl, P. M. Kort

We consider the optimal control problem of a firm which decides about investing into a capital stock needed for production. On the one hand the firm wants to maximize revenues, on the other hand it wants to minimize emissions which are caused by production.
To handle the conflicting objectives, we apply the epsilon-constraint method. A boundary value and continuation approach is used to numerically calculate the Pareto front for different initial state values. We are able to determine a threshold curve which separates areas on the Pareto front on which different long-run steady states are approached. We discuss differences and similarities to conventional Skiba points. Furthermore, we analyze the impact of key parameters on the solution paths and on the Pareto front.

Scalable Multilevel Domain Decomposition Solver for Immersed Boundary Finite Element Method

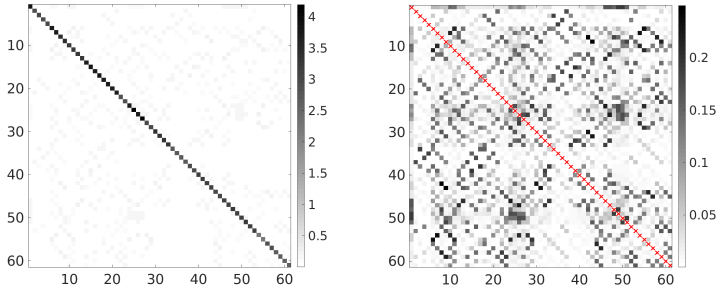
J. Šístek

Immersed boundary finite element method (FEM) presents an attractive approach to simulations avoiding the generation of large body-fitted meshes. This can be tedious and challenging for complex geometries as well as for very fine meshes distributed over a parallel computer and adaptively refined during a computation. However, the price to pay are more complicated formulations for the weak enforcement of Dirichlet boundary conditions, poor conditioning of stiffness matrices, and nonstandard numerical integration at the vicinity of the boundary.
We develop multilevel balancing domain decomposition by constraints (BDDC) method tailored to the solution of the linear systems arising in the context of immersed boundary FEM with parallel adaptive grid refinement. One crucial challenge is presented by load balancing the solver since the elements cut by the domain boundary require much more time for integration, whereas these elements have the same cost during the solution of the linear system as those fully inside the domain. Another challenge is presented by fragmenting of subdomains, which has two sources: i) the partitioning strategy based on a space-filling curve, and ii) extraction of the elements contributing to the stiffness matrix.
We present these concepts, the challenges, our implementation, and numerical results for the Poisson problem on complex geometries from engineering. This is joint work with Fehmi Cirak, Eky Febrianto, Matija Kecman, and Pavel Kůs.

Study of Sparsification Schemes for the FEM Stiffness Matrix of Fractional Diffusion Problems

D. Slavchev, S. Margenov

Anomalous diffusion describes various natural and social phenomena and processes in which the Brownian motion hypotheses are violated. Such problems can be modelled with the Fractional Laplace operator. In this work we consider the Finite Element discretization of the integral formulation of the Fractional Laplacian. The fractional diffusion operator is non-local. As a result the stiffness matrix $K \in \mathbb{R}^{n\times n}$ is dense. However, it can be observed that there are significant differences in the coefficients of K. For example, in a model problem in the computational domain $\Omega = [-1, 1] \times [-1, 1]$ is covered by an unstructured mesh with $n = 61$ nodes and a maximum element size $h = 0.3$, the diagonal entries of the stiffness matrix $K_{ii} \in [2.19, 4.19]$ while the off-diagonal elements have smaller absolute values $|K_{ij,i\neq j}| \in [0.2496, 0.0003]$. The structure of orders of magnitudes of the coefficients of K is shown on Fig. 1.



(a) All. (b) Without diagonal (marked with 'X').

Figure 1: Order of magnitude of the coefficients of the stiffness matrix.

We see that many of the off-diagonal coefficients have very small absolute values relative to the corresponding diagonal elements. In this work, we study sparsification techniques like removing or lumping (summing into the diagonal) the coefficients that fall under a specified threshold. In this way we construct sparse approximations of the stiffness matrix K. Numerical results for a model fractional Laplacian boundary value problem are presented. Based on them, the accuracy of the approximate solutions is analysed.

3D-1D Preconditioners for Inverse Problems Using Isogeometric Analysis

J. Sogn, K.-A. Mardal, M. Kuchta

Model reduction techniques are used in many applications ranging from groundwater wells to biological flows. When a completely monolithic approach is used, Lagrangian multipliers are introduced which are typically in a fractional Hilbert space. In this talk we consider a monolithic approach for a 3D-1D inverse problem where the Lagrangian multipliers are not in a fractional Hilbert space, however, the trade-off is that the 3D state space requires higher smoothness. We suggest a suitable preconditioner based on the operator preconditioning framework, then we discuss efficient realizations of this preconditioner and its robustness with respect to different

parameters such as diffusion constants, regularization parameters and discretization parameters. Since our approach requires higher smoothness, we use isogeometric analysis to obtain a conforming discretization.

An Inexact Block Factorization Precondioner for Incompressible Navier-Stokes Equations

S.-Z. Song, Z.-D. Huang

For a kind of 3×3 block structured linear equations related to the numerical solution of incompressible Navier-Stokes equations, based on the equivalent form of the system of linear equations, an inexact block factorization preprocessor is constructed. By obtaining an easier matrix similar to the preconditioned matrix, the upper and lower bounds of the real and imaginary parts of the eigenvalues of the preprocessed matrix are estimated based on Bendixson theorem. For uniform and stretchable meshs, numerical experiments show that compared with the existing ones, the constructed preconditioner is superior in the number of iteration steps and CPU time, and can make the GMRES a less dependent on the mesh size and the viscosity coefficient.

Fractional Diffusion Problems with Reflecting Boundaries

E. Sousa

Anomalous diffusive transport, described by fractional differential equations, arises in a large variety of physical problems. We consider a model that consists on the fractional diffusion equation subjected to reflecting boundary conditions. There has been a controversial discussion regarding the formulation of these boundaries, involving questions on what is the most appropriate boundary from the physical point of view. Therefore, we start to present different physical formulations regarding the boundaries. Then, numerical methods are proposed to determine the solutions of these diffusive models and it is shown how the presence of boundaries changes the general structure of the problem and of the numerical method, due to the non-locality of the problem. In the end, the influence of the different boundaries on the solutions is analysed.

Continuation Newton Methods with Applications to Plasticity

S. Sysala

This contribution arises from joint results with Professor Owe Axelsson and deals with continuation and adaptive Newton methods. These methods are applied and extended for purposes of computational plasticity where solvability may depend on the load. The aim is to find limit (critical) loads by parametrization of plastic problems. Consequently, one can define factors of safety and describe collapse states of structures. We illustrate the methods on examples dealing with stability of slopes or embankments.

An improved algorithm for Fredholm and Volterra integral equations

V. Todorov, S. Georgiev, S. Apostolv, I. Dimov

Integral equations are of high applicability in different areas of applied mathematics, physics, and engineering. In particular, they are widely used in mechanics, geophysics, electricity and magnetism, kinetic theory of gases, quantum mechanics, mathematical economics, and queuing theory. That is why it is reasonable to develop and study efficient and reliable approaches to solve integral equations. An important advantage of Monte Carlo methods is that they allow to find directly an unknown linear functional of the solution of integral equations with a number of operations necessary to calculate the solution of an integral equation only at one point of the domain. The existing Monte Carlo methods for integral equations are based on probabilistic representations of the Liouville-Neumann series for the second kind Fredholm integral equation. The possible unbiased approaches deal with infinite series, while the biased Monte Carlo approaches use probabilistic representations of truncated Liouville-Neumann series.
In the paper we propose an innovative approach for Fredholm integral equation and extend the Fredholm algorithm to Volterra equations. The approach uses the indicator function to transform the Volterra equation into Fredholm equation. The resulting Markov chains are inhomogeneous with an increasing absorption rate. Numerical examples for Freholm and Volterra integral equations with higher dimensions are given on basic reference problems and on high dimensional test cases. We also apply the Fredholm algorithm for large-scale problems of financial mathematics.

Optimization of the Standard Lattice Sequence for Multidimensional Integrals Regarding Large-Scale Finance Problems

V. Todorov, S. Georgiev, B. Chakarov, S. Hadziivanov

Lots of challenges in the multidimensional option pricing exist since this is one of the fundamental discipline in large-scale finance problems today. In this paper, for the first time we develop some new highly accurate lattice sequences, based on component-by-component construction methods: construction of rank-1 lattice rules with prime number of points and with product weights; construction of rank-1 lattice sequences with prime number of points and with product weight; construction of polynomial rank-1 lattice sequences in base 2 and with product weights. Our methods show significantly optimization compared to the results produced by the standard Monte Carlo algorithms and the most widely used lattice sequence. There is optimization in the relative error as well as the computational complexity and number of operation necessary to compute the arisen multidimensional integrals. The obtained results will play an extremely principal multi-sided role.

Improved Stochastic Lattice Methods for Large-Scale Air Pollution Model

V. Todorov, S. Georgiev, I. Dimov, R. Georgieva, T. Ostromsky

An important issue when large-scale mathematical models are used to support decision makers is their reliability. Sensitivity analysis of model outputs to variation or natural uncertainties of model inputs is very significant for improving the reliability of these models. By definition sensitivity analysis is a procedure for studying how sensitive are the output results of large-scale mathematical models to some uncertainties of the input data. It was not until recently that air pollution became a major global problem. It threatens whole ecosystems on Earth, having a vast impact on health and economy. A lot of effort is put into resolving the issue. There is still abundant interest in theoretical research too. One of the most powerful tools to do it is mathematical modelling.
In the study, a large-scale air pollution model is adopted, focusing on the Sobol approach for sensitivity analysis. We will use the advanced stochastic approach based on component by component construction methods. Optimized algorithms based on lattice rules have been designed and implemented, while their performance has been compared to the best available stochastic approaches, applied for multidimensional sensitivity analysis. Computations show signifiant improvement over the current stochastic methods. The obtained results would have an important multi-sided role.

Mean Field Games Planning Problems With General Initial And Final Measures

D. Tonon

The planning problem in Mean Field Games (MFG) was introduced by P.-L. Lions in his lessons, to describe models in which a central planner would like to steer a population to a predetermined final configuration while still allowing individuals to choose their own strategies. In a recent variational approach, see (Graber, Mészáros, Silva and Tonon 2019) and (Orrieri, Porretta and Savaré 2019) the authors studied the well-posedness of this problem in case of merely summable initial and final measures, using techniques, coming from optimal transport, introduced by Benamou and Brenier in 2000, extended to the congestion case in (Carlier, Cardaliaguet and Nazaret 2013), and already used to show the existence and uniqueness of weak solutions for classical MFGs by Cardaliaguet and collaborators. The case of less regular initial and final measures is now studied via techniques introduced by Jimenez in 2008, for the analogous problem in optimal transport.

Parallelisms of PG(3,4) with a Great Number of Regular Spreads

S. Topalova, S. Zhelezova

The problem: Let $\mathrm{PG}(n,q)$ be the n-dimensional projective space over the finite field $\mathbb{F}_q$. A *spread* in $\mathrm{PG}(n,q)$ is a set of mutually skew lines which partition the point set. A *parallelism* is a

partition of the set of lines by spreads. Parallelisms of the finite projective space PG(n, q) are of interest for problems from projective geometry, design theory, network coding, error-correcting codes, and cryptography. Parallelisms with a big number of regular spreads are of particular interest. All parallelisms of the smallest projective spaces PG(3,2) and PG(3,3) are known. Parallelisms of PG$(3, 4)$ which are invariant under automorphisms of orders greater than 2 have also been classified. Among them there are no parallelisms with more than 13 regular spreads (out of all 21 spreads). It has been proved that a regular parallelism (with 21 regular spreads) does not exist. To establish whether a parallelism with more than 13 regular spreads exists is an open problem.
Our contribution: The classification of all parallelisms of PG(3,4) which have automorphism groups of order at most 2 is presently infeasible. The nonclassified by now parallelisms with nontrivial automorphisms have an automorphism of order 2 fixing 5 spreads and upto isomorphism there are 776928 fixed parts of five spreads which must be extended to obtain all possible solutions. Since the extension of these solutions with all possible spreads is infeasible, we extend them with regular spreads only, namely this way we try to construct parallelisms which have at least 16 regular spreads. This way most of the fixed parts yield many partial solutions, but no full parallelisms. However, after extending all of them (by our own software run on the HPCS Avitohol) we finally find out that a parallelism of PG(3,4) with 16 regular spreads exists.

Circular Intuitionistic Fuzzy Knapsack Problem

V. Traneva, P. Petrov, S. Tranev

The Knapsack problem is an NP-hard combinatorial optimization problem whose objective is to find which of the given set of items with their value and weight to put in the knapsack to reach the highest possible total value without exceeding its capacity. Nowadays, there is great uncertainty in the parameters of this problem. Traditional methods for solving this problem cannot account for the uncertainty in the environment. In 2020, Atanassov introduced an extension of the Intuitionistic Fuzzy Set called the Circular Intuitionistic Fuzzy Set (C-IFS) to model the greater uncertainty of the environment.
This study suggests an index-matrix approach to a circular intuitionistic fuzzy knapsack problem (C-IFKP) in which all its parameters are circular intuitionistic fuzzy numbers by extending the classical dynamic optimization algorithm. The weights and values of a set of items are suggested by experts and their ratings are taken into account in the proposed algorithm. Software for performing the proposed circular intuitionistic fuzzy algorithm is also developed. The efficiency of the C-IFKP algorithm is applied to optimize the execution of the requests that an Ambulance team must satisfy in a certain time, taking into account the urgency of the request and its duration for execution. Three scenarios are proposed to the decision maker for the final choice - pessimistic, optimistic, and average.
The originality of the paper comes from the defined C-IFKP and the application of this algorithm to a problem for the efficient execution of requests by an ambulance team. The presented approach for the solution of C-IFKP can be applied to problems with imprecise parameters and can be extended to obtain the optimal solution for other types of C-IFKPs.

Discontinuous Galerkin Methods for Coupled and Compound Flood Simulations

E. Valseth, C. Dawson, C. Wichitrnithed,
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Recent tropical cyclones, e.g., Hurricane Harvey (2017), have lead to significant rainfall and resulting runoff with accompanying flooding. When the runoff interacts with storm surge, the resulting floods can be greatly amplified and lead to effects that cannot be modeled by simple superposition of its distinctive sources. Existing numerical models that incorporate both rainfall and riverine flows often consider surrogates to the SWE such as kinematic or diffusive wave approximations. However these are in many cases limited to flows found in inland regions as their assumption are too limiting in coastal regions. Coastal and storm surge models such as the ADvanced CIRCulation model (ADCIRC) based continuous Galekrin methods for shallow water equations (SWE) may have issues with mass balance due to their conservation properties. On the other hand, SWE solvers based on discontinuous Galerkin (DG) methods, such as those introduced previously avoid these issues due to their local mass conservation property. In this presentation, we present our latest advancements to our discontinuous Galerkin (DG) shallow water equation (SWE) solver as part of ongoing efforts in compound flood modeling for coastal domains. These advancements include rainfall onto the finite element mesh as well as river routing models by coupling our SWE solver to parametric rainfall models and inland hydrological models .

Strong Subregularity of Variational Inequalities: General Results and Case Studies

V. M. Veliov

Metric sub-regularity of mappings associated with variational inequalities (VIs) is a property that proved to be fundamentally important in the analysis of approximation methods for VIs, such as finite-dimensional approximations, gradient projection methods, Newton-type methods, etc. Such VIs arise, in particular, when considering the system of optimality conditions for control-constrained optimal control problems. The variables in the VIs in this case consist basically of the triples (*state function, co-state function, control function*). The choice of an appropriate (metric) space for the control function depends on the problem structure: L^2, L^∞, L^1 or other (not induced by norms) metric spaces are relevant for specific classes of problems. The talk will present new sufficient conditions for strong metric sub-regularity of VIs in (non-reflexive) Banach spaces, and, as application, several new result about sub-regularity of the Pontryagin optimality system for several classes of ODE or PDE optimal control problems.

Tensor-Train-Based Composite Algorithms For High-Dimensional Numerical Integration

R. G. Vuchkov, B. Alexandrov, G. Manzini, E. Skau, M. P. D. Truong

Numerical integration is a basic step in implementing complex numerical algorithms such as large-scale optimization. Specifically, numerical integration in PDE-constrained inverse problems can manifest as a building block in evaluating Finite Element Method integrals or as a critical component such as high-dimensional posterior distributions. The straightforward extension of a one-dimensional integration rule to a multi-dimensional grid by the tensor product of the spatial directions is practically infeasible beyond a relatively small number of dimensions due to the computational burden in terms of storage and number of arithmetic operations. The computational complexity scales exponentially with the number of dimensions.
The widely accepted solution to high dimensional integration is using Monte Carlo-type methods for sampling and integration. The tensor product approach for high-dimensional numerical integration, where we employ low-rank tensor-train representation of the integrand function. We present numerical evidence showing that our approach is competitive with the Monte Carlo method in terms of accuracy and computational costs up to several hundredths of dimensions while maintaining the expected convergence rate of the underlined quadrature rule, assuming enough regularity in the function to be integrated.

Application of Deep Kernel Models for Certified and Adaptive RB-ML-ROM Surrogate Modeling

T. Wenzel, B. Haasdonk, H. Kleikamp, M. Ohlberger, F. Schindler

In the framework of reduced basis methods (RB), we recently introduced a new certified hierarchical and adaptive RB-ML-ROM surrogate model, which can be used for efficient approximation of input-output maps that are governed by parametrized PDEs. This adaptive approach combines a full order model (FOM), a reduced order model (ROM) and a machine-learning (ML) model.
In the current presentation, we extend this method by leveraging novel kernel models for the machine learning part: On the one hand we make use of structured deep kernel models (SDKN), which put different classes of kernels into a structured multilayer setup. On the other hand we make use of two-layered kernel models, which can be viewed as machine learning hyperparameter optimized kernels, and use them in conjunction with greedy techniques.
We demonstrate the usablity of those enhanced kernel models for the RB-ML-ROM surrogate modeling chain and highlight their benefits in numerical experiments.

What about p?

R. Winther

The title of this talk refers to a question frequently asked by Ivo Babuška, from the late 1980s and on, following various talks on finite element methods. More precisely, *what can we say about the properties of finite element methods as we raise the polynomial degree?* Even today the so called p-method is less understood, and the corresponding analysis is less canonical, than the traditional approach of mesh refinement, i.e., the h-method. In recent years Rick Falk and I have developed a theory which represents a new tool to analyze finite element methods of high polynomial degree, which we refer to as *the bubble transform.* The key idea is to construct a decomposition into local bubbles which simultaneously covers all possible polynomial degrees. The purpose of this talk is to give a review of this theory, and to discuss potential applications.

Scalability of Extended Green Cloud Simulator

Z. Wrona, M. Paprzycki, M. Ganzha, S. Krzyżanowski

Recent years have seen an increase in interest in carbon-intelligent computing. In this context, the Green Edge Processing project inspired the development of the Extended Green Cloud Simulator (EGCS), which serves as an agent-based digital twin, facilitating the simulation of cloud infrastructure powered, in part, by renewable energy sources. Given that cloud systems must operate efficiently for a large number of clients, it was essential to evaluate the EGCS performance. Therefore, the following contribution briefly describes the design of the EGCS and discusses the results of the experimental assessment of its scalability.

On Block Version of the Randomized Kaczmarz Method

W.-T. Wu

For solving the large-scale systems of linear equations, the Kaczmarz method is a classic while effective iteration method and has been widely used in the area of signal and image processing. Its iteration is very simple and each iteration only utilizes one row of the coefficient matrix. Many works found that selecting the row in each Kaczmarz iteration randomly rather than sequentially can improve the convergence rate, but the convergence factor was difficult to be obtained until Strohmer and Vershynin proposed to choose the row randomly with probability proportional to its squared Euclidean norm and constructed the randomized Kaczmarz method in 2009. Utilizing more than one row of the coefficient matrix at each iteration can improve the convergence of the randomized Kaczmarz method. In this talk, we will discuss some block versions of the randomized Kaczmarz method, including their convergence analysis and numerical performances.

Learning Quadratic Hamiltonian Systems from the Data

S. Yildiz, P. Goyal, T. Bendokat, P. Benner

Hamiltonian systems intrinsically have several properties; among those, symplectic structure and energy preservation are essential properties. In this talk, we present data-driven modeling for nonlinear Hamiltonian systems. One of the key ingredients of our approach is the lifting principle. That is, sufficiently smooth nonlinear dynamics can be written as quadratic systems in a lifted coordinate system. We extend this principle of nonlinear Hamiltonian systems with a Hypothesis that nonlinear Hamiltonian systems can be transformed in another space via symplectic transformation so that the Hamiltonian of the transformed system can be a cubic function; this would then result in a quadratic system. Given data, we learn such a transformation using auto-encoder, which mildly enforces symplectic as well. Moreover, we discuss its extension to high-dimensional data. We illustrate the proposed methodology using various examples.

Part C

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