15th International Conference
June 16 - 20, 2025
Sozopol, Bulgaria

LARGE-SCALE SCIENTIFIC COMPUTATIONS LSSC'25

Scientific Program
Abstracts
List of Participants

Institute of Information and Communication Technologies
Bulgarian Academy of Sciences

PREFACE

The fifteenth International Conference on “Large-Scale Scientific Computations” LSSC 2025 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:

Pavel Bochev (Sandia National Laboratories, USA)
Ulrich Langer (Johannes Kepler University, Linz, Austria)
Kent-Andre Mardal (University of Oslo, Norway)
Markus Melenk (TU Wien, Austria)
Marcus Sarkis (Worcester Polytechnic Institute, USA)
Panayot Vassilevski (Portland State University, USA)
Gabriel Wittum (King Abdullah University of Science and Technology, Thuwal, Saudi Arabia)

LIST OF SPECIAL SESSIONS:

- Numerical Methods: Analysis and Computations, In memory of Raytcho Lazarov
  organized by Svetozar Margenov (IICT-BAS, BG), Panayot Vassilevski (Portland State University, USA)

- Mathematical and Numerical Modeling of Multiphysics Problems
  organized by Ivan Yotov (University of Pittsburgh, USA)

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

- Space-Time Methods for PDE-Based Simulation and Optimization
  organized by Ulrich Langer (Johannes Kepler University Linz, AT), Thomas Wick (Leibniz University Hannover, DE)

- Numerical Methods for Nonlocal Problems
  organized by Markus Faustmann (TU Wien, AT), Markus Melenk (TU Wien, AT)

- Fractional Operators and Multi-Physics
  organized by Timo Koch, Miroslav Kuchta, Kent-Andre Mardal (University of Oslo, Simula Research Lab, NO), Ludmil Zikatanov (Pennsylvania State University, USA)

- Recent Advances in Computational and Applied Poromechanics
  organized by Markus Bause (Helmut Schmidt University, Hamburg, DE), Johannes Kraus (University of Duisburg-Essen, DE), Maria Lymbery (University of Duisburg-Essen, DE)

- Mathematics and Algorithms for Predictive Digital Twins (DT)
  organized by Pavel Bochev (Sandia National Laboratories, USA), Irina Tezaur (Sandia National Laboratories, USA), Paul Kuberry (Sandia National Laboratories, USA)

- Adaptive and Robust Domain Decomposition Methods
  organized by Marcus Sarkis (Worcester Polytechnic Institute, USA)

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

- Large-Scale Models: from Life Sciences to Climate Research
  organized by Ivan Dimov (IICT-BAS, BG), Nevena Ilieva (IICT-BAS, BG)

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

- Numerical Solvers and Preconditioners for Differential Equations
  organized by Fabio Durastante (University of Pisa, IT), Mariarosa Mazza (University of Rome "Tor Vergata", IT)

- Porous Media Flow and Transport
  organized by Gabriel Wittum (KAUST, SA)

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

Media partnership

- Bulgarian Academy of Sciences
- Bulgarian Section of SIAM
- Algorithms, An Open Access Journal

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The organizers

June 2025

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Scientific Program[1]

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

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11:25 - 12:10	K.-A. Mardal, Mathematical Challenges of Modeling the Fluid Flow of the Brain - Brain Clearance, Sleep and Dementia

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Monday, June 16

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EXCURSION

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11:50 - 12:15	G. Nikolov, P.B. NIKOLOV, On the Error Bounds of the Gauss-Type Quadrature Formulae Associated with Spaces of Parabolic and Cubic Spline Functions with Double Equidistant Knots
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15:20 - 15:45	*Special Session on "Porous Media Flow and Transport"*
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15:20 - 15:45	M. KNODEL, A. Ngel, D. Logashenko, H. Zhao, A. Gehrke, A. Schneider, G. Wittum, Expansion of finite sized fractures in porous media with the ARTE algorithm
	Coffee Break
16:30 - 18:10	*Special Session on "Porous Media Flow and Transport"*
Chairperson	G. Wittum
16:30 - 16:55	R. WITTUM, A. Nägel, D. Logashenko, G. Wittum, Numerical Simulation of Phase Transitions for Saline Groundwater Flow in Soils with Permafrost
16:55 - 17:20	D. LOGASHENKO, A. Litvinenko, R. Tempone, G. Wittum, Numerical Simulation of Propagation of Uncertainties in Coastal Aquifers
17:20 - 17:45	S. LU, D. Logashenko, S. Matthai, A. Nägel, G. Wittum, Kinetic Multiphase Model And Full Coupled Implicit Scheme For Large-scale Subsurface Carbon Sequestration Simulation
17:45 - 18:10	A. SCHNEIDER, H. Zhao, D. Logashenko, J. Wang, A. Nägel, M. Knodel, G. Wittum, Modeling Groundwater Flow and Nuclide Transport in Fractured Media with d^3f++

19:30 **CONFERENCE DINNER**

Thursday, June 19

Parallel Sessions
Lecture Hall B

<u>14:30 - 15:45</u>	*Special Session on "Recent Advances in Computational and Applied Poromechanics"*
Chairperson	J. Kraus
14:30 - 14:55	L.T. Zikatanov, Neural Networks with Trainable Matrix Activation Functions
14:55 - 15:20	M. Hauck, A. Målqvist, A. Rupp, Iterative Methods For Large-Scale Elastic Graphs
15:20 - 15:45	Á. Pé de la Riva, F.J. Gaspar, X. Hu, J. Adler, C. Rodrigo, L. Zikatanov, On a Decoupled Solver for Biot's Model
	Coffee Break
<u>16:30 - 17:45</u>	*Special Session on "Recent Advances in Computational and Applied Poromechanics"*
Chairperson	J. Kraus
16:30 - 16:55	I. Yazici, I. Yotov, A Multipoint Stress-Flux Mixed Finite Element Method for the Biot System of Poroelasticity on Distorted Quadrilateral Grids
16:55 - 17:20	J. Lee, On Operator Preconditioning for Condensed Hybridized Systems
17:20 - 17:45	A. Borio, Virtual Element Methods and Mimetic Finite Differences for Simulations of Multiphase Flow and Poromechanics

19:30 **CONFERENCE DINNER**

Thursday, June 19

Parallel Sessions
Lecture Hall C

14:30 - 15:45	*Special Session on "Space-Time Methods for PDE-Based Simulation and Optimization"*
Chairperson	U. Langer
14:30 - 14:55	H. Fischer, V. Kosin, J. Roth, J.P. Thiele, T. WICK, Space-Time Modeling, Discretization, And Goal-Oriented Error Estimation of Coupled Problems
14:55 - 15:20	V. KOSIN, A. Fau, F. Hild, T. Wick, Dual-Weighted Residual Goal-Oriented Error Estimation For Space-Time Adaptivity In Phase-Field Fracture
15:20 - 15:45	B. ENDTMAYER, U. Langer, A. Schafelner, Goal-Oriented Adaptive Space-Time Finite Element Methods for the Parabolic p-Laplace Equation
	Coffee Break
16:30 - 17:45	*Special Session on "Space-Time Methods for PDE-Based Simulation and Optimization"*
Chairperson	M. Bause
16:30 - 16:55	T. Führer, G. GANTNER, M. Karkulik, Space-Time FEM-BEM Couplings for Parabolic Transmission Problems
16:55 - 17:20	L. Diening, R. Stevenson, J. STORN, A Quasi-Optimal Space-Time FEM With Local Mesh Refinements For Parabolic Problems
17:20 - 17:45	M. ZANK, A Space-Time Continuous Galerkin Finite Element Method for Linear Schrödinger Equations

19:30 **CONFERENCE DINNER**

Thursday, June 19

Parallel Sessions
Lecture Hall D

<u>14:30 - 15:45</u>	*Special Session on "Variational Analysis and Optimal Control"*
Chairperson	R. Ferretti
14:30 - 14:55	M. Krastanov, N. RIBARSKA, Non Degeneracy of Optimality Conditions
14:55 - 15:20	T. Tsachev, I. VASSILEVA, Policies to Curtail the Size of the Informal Sector in an Economy with Fiscal Rules
15:20 - 15:45	M. IVANOV, M. Krastanov, N. Ribarska, Differential Inclusions and Quasi-Lyapunov Functions
	Coffee Break
<u>16:30 - 17:20</u>	*Special Session on "Variational Analysis and Optimal Control"*
Chairperson	N. Ribarska
16:30 - 16:55	M.I. Krastanov, R. Rozenov, B.K. STEFANOV, Constrained Infinite-Time Horizon Linear Quadratic Optimal Control under Uncertainty
16:55 - 17:20	M. Borisov, N. Dimitrova, M. KRASTANOV, On a Two-Stage Anaerobic Digestion Model

19:30 **CONFERENCE DINNER**

Friday, June 20

Parallel Sessions
Lecture Hall A

<u>09:00 - 10:15</u>	*Contributed Talks*
Chairperson	S. Harizanov
09:00 - 09:25	B. LAZAROV, M. Schmidt, Large Scale Parallel Topology Optimization of Time Harmonic Dynamic Problems
09:25 - 09:50	N. KOSTURSKI, S. Margenov, Y. Vutov, Non-overlapping DD-BURA Preconditioning on Unstructured Tetrahedral Meshes
09:50 - 10:15	D. SLAVCHEV, N. Kosturski, S. Harizanov, Practical Application of BURA to Fractional Diffusion Problems with Power Outside of the Unit Interval
	Coffee Break
<u>10:45 - 12:00</u>	*Contributed Talks*
Chairperson	A. Andreev
10:45 - 11:10	A.B. Andreev, M.R. RACHEVA, Mixed Finite Element Approximation for Sixth-order Eigenvalue Problem
11:10 - 11:35	A.Z. Atanasov, M.N. Koleva, L.G. VULKOV, Numerical Source Determination in a Space Fractional Parabolic Equation of Lévy Flights of Honeybee in Search of Foods
11:35 - 12:00	M.N. KOLEVA, L.G. Vulkov, Numerical Identification of Time-dependent Source in a Quasilinear Parabolic Equation

Lecture Hall C

<u>09:00 - 10:15</u>	*Special Session on "Space-Time Methods for PDE-Based Simulation and Optimization"*
Chairperson	G. Gantner
09:00 - 09:25	M. BAUSE, Space-Time FEM for the Navier–Stokes System: Discretizations, Solver and Analysis
09:25 - 09:50	M. REICHELT, O. Steinbach, Space-Time Finite Element Methods in Thermo-Elastodynamics
09:50 - 10:15	H. Egger, A. SCHAFELNER, A Fixed-Point Iteration for Nonlinear Time-Periodic Parabolic Problems

Friday, June 20

Parallel Sessions
Lecture Hall D

<u>09:00 - 10:15</u>	*Special Session on "Applications of Metaheuristics to Large-Scale Problems"*
Chairperson	S. Fidanova
09:00 - 09:25	A. Badica, C. BADICA, M. Ganzha, M. Paprzycki, Y. Watanobe, Optimization of Tensor Train Contraction
09:25 - 09:50	P. ZHIVKOV, V. Todorov, Sensitivity Analysis of Volume Spread Analysis-Based Trading Algorithms Using Monte Carlo Simulation
09:50 - 10:15	L.M. LASKOV, M.M. Marinov, Polynomial Algorithm for Minimum Complete Pareto Front of a Biobjective Minimum Spanning Trees Problem
	Coffee Break
<u>10:35 - 11:50</u>	*Special Session on "Applications of Metaheuristics to Large-Scale Problems"*
Chairperson	L. Laskov
10:35 - 11:00	V. TODOROV, S. Apostolov, P. Zhivkov, S. Fidanova, I. Dimov, MEfficient Monte Carlo Solutions for High-Dimensional Fredholm Integral Equations
11:00 - 11:25	V. Todorov, B. CHAKAROV, S. Hadzhiivanov, M. Chechev, Y. Dimitrov, Intelligent Simulation-Based European Option Valuation
11:25 - 11:50	V. Todorov, V. Traneva, S. Tranev, Y. DIMITROV, S. Apostolov, Refined Stochastic Methods for Large Linear Algebraic Systems

Part B

Abstracts[2]

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

Numerical treatment of Riesz-Feller operators using hp-FEM

F. Achleitner, C. Kuehn, M. Melenk, A. Rieder

In this talk, we present a numerical scheme for discretizing non-symmetric Riesz-Feller operators on $\mathbb{R}$. Given parameters $\alpha \in (0,2)$ and $|\theta| \leq \max(|\alpha|, 2-|\alpha|)$, these operators are characterized by the Fourier symbol

$$D^\alpha_\theta f := \mathcal{F}(\psi^\alpha_\theta(\xi)\mathcal{F}[f]) \qquad \text{with} \qquad \psi^\alpha_\theta(\xi) := -|\xi|^\alpha e^{i\mathrm{sign}(\xi)\theta\frac{\pi}{2}}$$

and generalize the usual fractional Laplacian for $\theta \neq 0$.
The discrete scheme is based on a representation of D^α_θ as the Dirichlet-to-Neumann map of a degenerate non-symmetric elliptic system in $\mathbb{R} \times (0, \infty)$. This system is then discretized using *hp* finite elements on a finite cylinder. We present numerical analysis of such schemes for elliptic problems and talk about practical considerations, for example when using such a scheme in the context of the fractional Allen-Cahn equation.

Machine-Learned Correction Towards 3D Radiative Transfer for Climate Models

J.A. Actor, J. Torchinsky, B. Hillman

Radiation effects and radiative transfer (RT) have an outsized role in the accuracy of global climate models; however, such computations are often among the most expensive components of atmospheric models. To make such models tractable, most large-scale codes use simplified RT equations that assume radiation only propagates in one dimension. While this assumption is sufficient for coarse simulations, atmospheric models' resolution have improved to the point where this approximation begins to break down. To solve this problem, we build a novel machine-learned correction to map 1D RT results to a full 3D model. To do so, we generate a novel set of high-resolution atmospheric states for both 1D RT and 3D RT models, and then build a constrained machine learning problem where a corrector is learned to obey the full 3D RT equations:

$$\begin{aligned}\widehat{s} \cdot \nabla_x u(x, \widehat{s}) + \beta_\epsilon(x) u(x, \widehat{s}) - \beta_\epsilon(x)\omega(x) \int_{\mathbb{S}^2} \phi(\widehat{s}, \widehat{s}')u(x, \widehat{s}'d\widehat{s}' \\ = \beta_\epsilon(x)(1-\omega(x))B(x, \widehat{s}),\end{aligned}$$

for position $x \in \Omega \subset \mathbb{R}^3$ and RT direction $\widehat{s} \in \mathbb{S}^2$. Due to the high-dimensional setting of the RT equations, we use radial basis functions (RBFs) to represent the basis for our machine learning problem; the shape parameters are informed by training on data, with constraints so that the RBFs are properly defined on the domain $\Omega \times \mathbb{S}^2$. We demonstrate the effectiveness of this new machine learning scheme for this problem, highlighting the accuracy and generalization capabilities of our model for RT equations used in modern climate models.

Mixed Finite Element Approximation for Sixth-order Eigenvalue Problem

A.B. Andreev, M.R. Racheva

This paper deals with a sixth-order adjoint Sturm-Liouville problem. The mixed finite element method is considered, with the main objective being to obtain an approximation using piecewise linear polynomials. Variational aspects are discussed and error estimates are given for the approximate eigenvalues and eigenfunctions. Numerical results are also presented.

Linear Estimates for Trajectories of a State-constrained Differential Inclusions

S. Apostolov, M. Krastanov, N. Ribarska

We consider differential inclusions $\dot{x} \in F(x)$ for Lipschitz set-valued map $F : \mathbb{R}^n \rightrightarrows \mathbb{R}^n$ with phase constraint closed set $K \subset \mathbb{R}^n$, i.e. we are interested in solutions of the inclusion, whose values belong to the set K. Let $\mathcal{C}$ denote the solution of the inclusion, i.e. the set of pairs $(x, y) \in L^\infty \times L^1$ such that $\dot{x} = y$ and $y \in F(x)$. Let $\mathcal{K}$ denote the set of pairs $(x, y) \in L^\infty \times L^1$ such that the values of x belong to K. Let $(\bar{x}, \dot{\bar{x}}) \in \mathcal{C} \cap \mathcal{K}$. Our main goal is to show that under some additional hypothesis on K, the sets $\mathcal{C}$ and $\mathcal{K}$ are subtransversal at $(\bar{x}, \dot{\bar{x}})$. Unraveling the definition of subtransversality, this essentialy means, that there exists a constant M such that given an element $(x, \dot{x}) \in \mathcal{C}$ which is close enough to $(\bar{x}, \dot{\bar{x}})$, there exists an element of $(y, \dot{y}) \in \mathcal{C} \cap \mathcal{K}$ for which $\operatorname{dist}((x, \dot{x}), (y, \dot{y})) \leq M \operatorname{dist}((x, \dot{x}), \mathcal{K})$. The distances here are taken with respect to the natural norm in $L^\infty \times L^1$.
Similar linear estimates do exist in the literature, although they do not seem to put the problem in the context of subtransversality of sets. The known results give similar linear estimates when the set K has smooth enough boundary, or when it is convex. We aim to relax this assumptions.

Mixed Finite Element Projection Methods for the Unsteady Brinkman Equation

C. Aricó, R. Helmig, I. Yotov

The Brinkman equation finds many applications when the porous media present heterogeneous porosity/permeability values, in such a way that in some portions of the domain the flow is governed by the Darcy's law and elsewhere by the Stokes equation. We present a $H(\text{div})$-conforming mixed finite element methods for the solution of the

unsteady Brinkman equation, assuming the porous medium saturated by a single-phase incompressible fluid. One of the main issues in the the numerical solution of the incompressible Stokes or Brinkman equations is related to the solution of a saddle point problem, where the pressure plays the role of a Lagrange multiplier to obtain the divergence-free constraint. We propose a projection method in the framework of the incremental pressure correction method, where a predictor and a corrector problem are sequentially solved (PP and CP, respectively), accounting for the viscous effects and incompressibility, respectively. A stress-velocity and a velocity-pressure mixed formulation are used in the PP and CP, respectively. In the implementation we focus on generally unstructured simplicial grids. We use a second order multipoint flux mixed finite element method based on the Raviart-Thomas space RT_1 and a suitable quadrature rule. In the PP this approach allows for a local stress elimination, resulting in element-based systems for each velocity component. In the CP, the velocity is locally eliminated and an element-based system for the pressure is solved. At the end of each time step we obtain a second order accurate $H(\mathrm{div})$-conforming piecewise linear and pointwise divergence free velocity. The algorithm requires solving at each time step three (in 2D) or four (in 3D) symmetric positive definite systems, two (in 2D) or three (in 3D) for the components of the predicted velocity, in the PP, and one for the pressure, in the CP. Due to the local elimination of the viscous stress and the corrected velocity, the systems have only three (in 2D) or four (in 3D) unknowns per element, which results in a very computationally efficient algorithm, with a significant reduction from the original saddle point systems. We present a series of numerical tests to show the performance of the proposed method.

Numerical Source Determination in a Space Fractional Parabolic Equation of Lévy Flights of Honeybee in Search of Food

A.Z. Atanasov, M.N. Koleva, L.G. Vulkov

Based on recent experimental engineering, some authors proposed Levy-flight diffusion models to predict transgenic pollen dispersal. In this paper, we study a space-fractional inverse problem for source determination with a final-time measurement, modeling the flight of a honeybee in search of food. This ill-posed inverse problem is reduced by Tikhonov regularization algorithm to a well-posed direct problem. Then, it is solved by weighted difference scheme with second order of accuracy in space. Results from computational test examples are presented and discussed.

A Comparative Analysis of the Effects of Skipping and Leaping in Sobol and Halton Sequences

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

Sobol and Halton sequences are widely used low-discrepancy sequences in numerical simulations. They offer superior uniformity over pseudorandom numbers and are particularly

effective in numerical integration, optimization, and high-dimensional simulations. In practice, they are usually scrambled to improve their effectiveness, allow for statistical error estimation, and avoid certain artefacts. Various scrambling constructions are known and used for both sequences, with a trade-off between complexity, computational time requirements, and uniformity properties. Both Sobol and Halton sequences allow for using "skip" and "leap" parameters in their construction. This study compares the effects of varying the skip and leap parameters on the effectiveness of the scrambled Sobol and Halton sequences in applications. The numerical experiments are conducted to construct a Markov chain to estimate the maximum eigenvalue of symmetric matrices via Sobol and Halton sequences. The results show that changes in the skip and leap parameters influence the solution of the given problem. Based on our analysis, we propose strategies for solving large-scale scientific problems using Sobol and Halton sequences with specific skip and leap parameters when using MPI and CUDA for parallel computing.
Acknowledgments: The work of the authors (S.-M. Gurova and T. Gurov) was supported by the National Geoinformation Center (part of the National Roadmap for Research Infrastructures) through grant No. D01-321/30.11.2023, funded by the Ministry of Education and Science of the Republic of Bulgaria.

Novel Algorithm for Adaptive Circuit Construction for Quantum Kernel Methods

E. Atanassov, A. Karaivanova, S. Yordanov, S. Spasov,
M. Durchova, A. Kirilov

Quantum Computing attracted significant attention, partially due to the potential to achieve significant speedups in diverse optimization tasks. Quantum Machine Learning aims to utilize quantum computations as part of the workflow, in my cases resulting in hybrid methods. Kernel methods are well studied approach in problems for classification or regression, where kernels are employed to deal with non-linearity in the data. Kernels that use quantum circuits have been considered, and some theoretical or practical results have been achieved. As we have the flexibility to choose how to construct the basic quantum circuit to be used, the question is how to dynamically build a circuit that is sufficiently adapted to the dataset. In this work we propose a novel algorithm that uses genetic algorithms for this task, while also employing a neural network in order to speed-up the evolutionary process by attempting to predict the accuracy of the kernel method when using a candidate circuit. We describe in detail the algorithm and provide numerical examples using widely known datasets that show the performance that can be obtained. We demonstrate that the method is viable and produces results that are comparable to other established prediction algorithms, with wide potential for further improvement.

Basic Preconditioners for Some Kernel Methods

B. Ayuso de Dios, L. Rosasco, G. Vitale

Kernel methods provide an elegant and often effective framework to design algorithms for non-linear, non-parametric learning. However, at least in their basic form, the resulting schemes become unfeasible when dealing with large datasets due to computational requirements in terms of time and especially memory. Overcoming these drawbacks has prompt an upsurge of research in the design of several computational strategies for large scale kernel method. To alleviate the memory limitation some kind of Randomization is typically used. In this talk we consider the solution to a Kernel Ridge Regression (Least squares) problem. Taking inspiration from the Domain Decomposition techniques for preconditioning PDEs we develop some simple solvers for the solution of the corresponding linear system. The resulting solution strategies combine ideas of subspace correction methods with the use of randomised projections. Extensive numerical results show the viability of the proposed solvers. The talk is based on a collaboration with L. Rosasco (U. Genova) and G. Vitale (U. Milano-Bicocca).

Optimization of Tensor Train Contraction

A. Badica, C. Badica, M. Ganzha, M. Paprzycki, Y. Watanobe

Tensors are abstract mathematical objects with many applications in science and engineering. In computational science, tensors are defined as generalizations of matrices from bi-dimensional to multi-dimensional case. Tensors can be in- terconnected in graph-like structures known as tensor networks that are used for modeling complex systems in science and engineering. Tensor networks allow the modeling of systems composed of many locally interacting components. Such models are typically encountered in physics and machine learning for capturing states of quantum systems and neural network computations. Tensors suffer from the “curse of dimensionality”, i.e. the representation of tensors requires exponential memory in the number of tensor dimensions (also known as tensor rank). Therefore, applications are based on low-rank factor- ization of tensors, known as tensor decomposition. There are many kinds of tensor decomposition and all of them are actually special types of tensor net- works. A tensor decomposition is learned and processed using specialized tools for manipulating tensor networks. Tensor decomposition offers great potential for more efficient tensor representation supporting high-performance parallel and distributed processing. Specialized tensor networks include tensor trains (also known as matrix prod- uct states – MPS), tree tensor networks, and square tensor networks (also known as projected entangled pair states – PEPS). While optimal contraction of tensor networks is known to be generally NP-hard, it attracted the research interest by focusing on exhaustive and heuristic algorithms. Tensor contraction is a tensor operation that occurs in many applications of tensor networks. Optimal tensor contraction is known to be generally NP-hard. One particular type of tensor network is the tensor train. In this paper we show that tensor train contraction is a generalization of matrix chain multiplication from bi-dimensional to multi-dimensional matrices. We propose a polynomial dynamic programming algorithm for optimal tensor train contraction and we sketch its implementation

High Order Methods for Fractional Diffusion

B. Bahr, C. Marcati, M. Faustmann, J.M. Melenk, C. Schwab

For the Dirichlet problem of the integral fractional Laplacian in a polygon Ω and analytic right-hand side, we show exponential convergence of the *hp*-FEM based on suitably designed meshes, [Faustmann, Marcati, Melenk, Schwab, 2023]. These meshes are geometrically refined towards the edges and corners of Ω. The geometric refinement towards the edges results in anisotropic meshes away from corners. The use of such anisotropic elements is crucial for the exponential convergence result. These mesh design principles are the same ones as those for *hp*-FEM discretizations of the Dirichlet spectral fractional Laplacian in polygons, for which recently exponential convergence also has been established, [Banjai, Melenk, Schwab 2023]
The *hp*-FEM convergence result relies on the recent work [Faustmann, Marcati, Melenk, Schwab 2022], where weighted analytic regularity of the solution is shown in a way that captures both the analyticity of the solution in Ω and the singular behavior near the boundary. Near the boundary the solution has an anisotropic behavior: near edges but away from the corners, the solution is smooth in tangential direction and higher order derivatives in normal direction are singular at edges. At the corners, also higher order tangential derivatives are singular. This behavior is captured in terms of weights that are products of powers of the distances from edges and corners.
We will also address the issue of setting up the stiffness matrix. We show that a judicious combination of Duffy-like transformations and hp-quadrature techniques allow one to set up the matrix with work growing algebraically in the problem size while retaining the exponential convergence of *hp*-FEM. The emphasis will be placed on the 1D fractional Laplacian, [Bahr, Faustmann, Melenk, 2024].

Reduced Order Modeling for a Poroelastic Media with Faults

E. Ballini, A. Cominelli, L. Dovera, L. Formaggia,
A. Fumagalli, A. Scotti, P. Zunino

Subsurface exploitation projects, including CO2 storage, require computationally expensive simulations to assess fluid transport and fault stability, often coupling porous media flow with mechanics. To reduce costs, we propose using deep learning reduced-order modeling (DL-ROM), where an autoencoder identifies a reduced space based on high-fidelity simulations. The model incorporates uncertainties like Young's moduli, permeabilities, fault transmissibility, and process controls such as CO2 injection rates.

DL-ROM is applied to synthetic CO_2 storage scenarios featuring sloping faults at risk of destabilization. High-fidelity simulations use finite volume-based commercial software for fluid flow and finite element or PorePy for mechanical analysis. The surrogate model demonstrates accuracy and efficiency, reproducing fault stress states and enabling rapid multi-query analyses for statistical fault stability assessments, marking a novel use of DL-ROMs in this context.
To reproduce also the two-phase flow with DL-ROMs, first we address the complexity associated with the presence of fractures or faults along with counter-current flows driven by gravity and pressure gradients. A mixed-dimensional approximation alleviates the computational burdens, while hybrid upwinding improves stability and convergence of non-linear solvers. Tested across varied flow regimes and geometries, this approach enhances solver performance significantly, particularly in reducing Newton iterations.
Having the high-fidelity simulations, we further extend DL-ROMs to two-phase flow, accommodating rock and flow properties. Using DL-ROM in a mixed-dimensional framework, we efficiently perform tasks like sensitivity analyses and inverse problem-solving, achieving promising accuracy and speed for complex systems.

Space-Time FEM for the Navier–Stokes System: Discretizations, Solver and Analysis

M. Bause

Space-time finite element methods (STFEMs) feature the natural construction of higher order discretization schemes for partial differential equations. They offer the potential to inherit most of the rich structure of the continuous problem, while maintaining stability, and achieve accurate results on feasible grids. The solution of the algebraic systems is a challenging task.
Firstly, we present our STFEMs for simulating in three space dimensions solutions to the Navier–Stokes equations. **Arbitrary order** discontinuous Galerkin methods for the time discretization and inf-sup stable finite element pairs with discontinuous pressure for the space discretization are applied in a local (time stepping) approach. For solving the Newton linearized algebraic systems, GMRES iterations with **Geometric Multigrid Preconditioning** based on a **local Vanka smoother** are applied. Finally, the combination of the methods with duality based **a posteriori error control (DWR approach)** and mesh adaptivity is addressed. This is a joint work with M. Anselmann, M. P. Bruchhäuser and N. Margenberg.
Secondly, we address the optimal order approximation of the pressure trajectory for an **equal-order in time** and **continuous in time variational discretization** of velocity and pressure. In the literature, the pressure approximation of (Navier-)Stokes systems has attracted less attention than the velocity approximation, even though being of equal importance for applications, for instance, for the computation of the drag and lift coefficient of flows around obstacles. Difficulties in the pressure approximation arise from the saddle point structure of the Stokes system and the lack of information regarding the computation of discrete initial pressure values. For simplicity, the Stokes system and a

piecewise linear approximation in time are studied here. By collocation techniques, we propose a post-processed pressure in the set of the pressure solutions which guarantees for the **pressure error** in the L^2-norm **optimal** second order **estimates** in time and optimal order estimates in space. This is a joint work with G. Matthies and F. Schieweck.

On Low-Dimensional Approximation of Function Spaces of Interior Regularity

M. Bebendorf

Interior regularity is a property that is satisfied by the solutions of many elliptic second order boundary value problems. Spaces of functions satisfying this property can be approximated by suitable exponentially convergent finite-dimensional approximation spaces. We present a new efficient generalized finite element method that is able to exploit this in the case of linear problems.

Efficient Solvers for Linear Poroelasticity with Application to Parameter Estimation

M. Béreš, S. Berešová, T. Luber

This work presents recent advances in modeling and solving linear poroelasticity problems, applied to the Tunnel Sealing Experiment, conducted in an underground research laboratory. Our ultimate goal is to estimate the material parameters of the rock massif using experimental data, employing a Bayesian inversion framework augmented by surrogates. This framework requires evaluating thousands of instances of the forward poroelastic model with varying material parameters.
The poroelastic model, implemented in FEniCSx, incorporates pore pressure and displacement dynamics governed by Biot's equations. It is discretized using the finite element method in space and the implicit Euler method in time. Efficient and fast solving of this model is critical for the effective application of the Bayesian framework.
To address this, we tested block preconditioners and splitting methods for solving timestep problems with heterogeneous parameters. These were combined with deflated Krylov methods, which exploit similarities between problems with modified parameters. Employing these methods significantly accelerated the computation, resulting in more samples being computed and consequently leading to a better fit of the physical parameters.

Localization of Fractional Norms and Applications to Domain Decomposition

S. Bertoluzza

We present some novel localization results for fractional norms of both positive and negative order, and show how, in the framework of domain decomposition methods, such results can be exploited, on the one hand, to design computationally efficient natural norm stabilization terms for unstable non conforming discretizations, and, on the other hand, to derive preconditioners which are fully robust with respect to the order of the discretization method.

Analysis of a Class of Problems Involving Impulsive Lotka–Volterra Control Systems

P. Bettiol, P. Bruneau, J. Rouot

Recent mathematical models in ecology, based on the seminal contributions of Lotka and Volterra, describe the population dynamics of interacting species. These models have recently been validated through experiments on mice aimed at reducing infections by a pathogenic agent, framed within optimal control problems.
The control system involves two types of treatments. Non-invasive treatments are modeled as permanent controls, represented by measurable functions corresponding to interventions like probiotics and antibiotics. On the other hand, invasive treatments are described using impulsive controls, representing interventions such as transplantation and fecal injections.
This presentation examines a general Lotka–Volterra control system that incorporates both continuous and impulsive controls. The impulsive control is modeled as an atomic measure, allowing state trajectories to exhibit discontinuities at a single jump time, which is treated as a free variable. The objective of the problem is to minimize the cost associated with the size of the jump in the state trajectory, while ensuring that the endpoints of the trajectories lie within a prescribed closed set.
The problem is studied from two perspectives. The first approach uses the optimal multiprocess framework to derive necessary optimality conditions. The second approach replaces the atomic measure with a regular, Borel, nonnegative-valued measure. Assuming that the minimizer corresponds to an atomic measure, we derive the necessary optimality conditions and compare them to the ones obtained from the first approach. Notably, the first approach yields sharper transversality conditions, while the second approach provides an additional condition in the form of an inequality involving the multipliers and the state variable over time.
Building on these theoretical results, we then introduce a two-step numerical scheme that combines both direct and indirect methods to effectively solve the optimal control problem. This scheme is subsequently applied to a generalized Lotka–Volterra model.

Linearization of Differential Inclusions

M. Bivas, M.I. Krastanov, N. Ribarska

We extend the approach of Dubovickiĭ and Miljutin for linearization of the dynamics of smooth control systems to a non-smooth setting. We consider dynamics governed by a differential inclusion and we study the Clarke tangent cone to the set of all admissible trajectories starting from a fixed point. Our approach is based on the classical Filippov's theorem and on the important property "subtransversality" of two closed sets.

Data-driven Compact Models for Devices and Circuits: a System Identification Approach for Non-intrusive Reduced Order Modeling of Normal and Radiation Environments in Microelectronics

P. Bochev, J. Hanson, E. Thieme, T. Meissner, P. Kuberry, B. Paskaleva, L. Musson

We demonstrate that system identification (SysID) techniques can provide basis for effective, non-intrusive Reduced Order Modeling (ROM) in microelectronics. The first part of the talk will focus on the development of ROMs for semiconductor devices with particular emphasis on radiation effects. Our approach is based on state-space gray box architectures in which the state equation is informed by a mathematical model of an idealized semiconductor device. Development of these gray box ROMs does not require snapshots of the internal state, nor does it require access to the discretized equations as in traditional projection-based ROM. To illustrate the approach we train gray box photocurrent models for a Zener diode and a BJT device using experimental and synthetic data, and compare them with traditional compact analytic models and black box neural network models.

In the second part of the talk we consider ROMs for common circuits, such as operational amplifiers, comparators, and voltage regulators, that are key building blocks in microelectronics. Our SysID approach is motivated by the fact that these circuits operate in a primarily memoryless capacity, and exhibit simple "scripted" behaviors even though their transistor-level descriptions may have rather complex nonlinear mathematical structures. We show that such circuits can be mapped to model architectures, such as the canonical Hammerstein architecture, that are sufficiently expressive to capture their characteristic behaviors, yet remain simple enough to escape the computational and calibration burdens that stem from the excessive expressivity of universal model architectures. The talk will conclude with a brief discussion of circuit ROMs based on Sparse Identification of Nonlinear Dynamical systems (SINDy) and select simulation results with our SysID circuit models.

Decoupled Solution Methods for Multiphysics Problems Based on Dynamic Interface Flux Surrogates

P. Bochev, R. Pawar, P. Kuberry, J. Owen, E. Huyhn, J. Connors

Digital twin (DT) modelling, simulation, and data assimilation tasks often require numerical solution of complex multiphysics system models comprising many heterogeneous components. Decoupled, or partitioned solution methods for such models can significantly improve the efficiency of DT workflows. Typically, decoupled methods employ data transfers between the constituent physics components to synchronize them and enable their independent solution. By treating each subproblem as a separate entity, these methods enable code reuse, increase concurrency and provide a convenient framework for plug-and-play multiphysics simulations. However, accuracy and stability of partitioned methods depends critically on the type of information exchanged between the subproblems. The exchange mechanisms can vary from minimally intrusive remap across interfaces to more accurate but also more intrusive and expensive estimates of the necessary information, such as dual Schur complements or variational flux recovery techniques. Data-driven system identification techniques provide an opportunity to close the accuracy, performance and intrusiveness gaps between these exchange mechanisms by enabling the construction of accurate, computationally efficient and minimally intrusive data transfer surrogates. This approach shifts the principal computational burden to an offline phase, leaving the application of the surrogate as the sole additional cost during the online simulation phase. To demonstrate the approach, we consider the problem of diffusive transport of a scalar quantity across an interface separating two different materials. In the offline phase we use training data generated by simulating this problem with appropriately chosen initial conditions to learn small dynamical systems approximating the evolution of the interface flux. In the online, simulation phase, we use these dynamic flux surrogates to estimate the flux exchanged between the subdomains for arbitrary initial conditions. We discuss several different strategies for learning the flux surrogates, such as Dynamic Mode Decomposition (DMD) and Operator Inference. Numerical results confirm that the computational cost of the resulting decoupled scheme is comparable to that of a traditional loosely coupled partitioned method, while its accuracy is significantly higher.

Multigrid Preconditioning for FD-DLM Method in Elliptic Interface Problems

N. Alshehri, D. Boffi, C. Chaoveeraprasit

We investigate the performance of multigrid preconditioners for solving linear systems arising from finite element discretizations of elliptic interface problems using the Fictitious Domain with Distributed Lagrange Multipliers (FD-DLM) formulation. Numerical experiments are conducted using continuous and discontinuous finite element spaces for the Lagrange multiplier. Results indicate that multigrid is a promising preconditioner for problems in the FD-DLM formulation.

Optimal Control of Multiagent Systems with Aggregation

M. Bonafini, G. Cavagnari, A. Marigonda

We investigate, both in the Lagrangian and in the Eulerian framework, a two-scale dynamics governing a multi-agent system. Multi-agent systems can be described as systems where a multitude of identical interacting agents move. A statistical description of these systems naturally leads to a two-scale dynamics, where the microscopical scale describes the motion of each agent, possibly influenced by the distribution of all the others, and the macroscopical scale describes the evolution of the overall distribution.
In this talk, we present some recent results concerning tools used to study optimization problems in this setting, together with an application to a resources harvesting problem, generalizing some ideas from branching optimal transportation theory. The results have been obtained in collaboration with M. Bonafini and A. Marigonda (University of Verona, Italy).

Virtual Element Methods and Mimetic Finite Differences for Simulations of Multiphase Flow and Poromechanics

A. Borio

Simulations of underground phenomena in real scenarios can be limited or slowed down by meshing issues. New generation numerical methods such as Mimetic Finite Differences (MFD) and Virtual Element Methods (VEM) can help circumventing such issues, since they allow the use of general polyhedral meshes and deal seamlessly with aligned faces.
We present some recent advancements in the simulation of compositional multiphase flow and poromechanics using VEM and MFD, targeting the simulation of CO2 injection in the subsoil on general polyhedral meshes. Simulations are done using GEOS, an open-source, multiphysics simulator developed cooperatively by Lawrence Livermore National Laboratory, Stanford University, TotalEnergies, and Chevron.

On a Two-Stage Anaerobic Digestion Model

M. Borisov, N. Dimitrova, M. Krastanov

The dynamics of a two-stage anaerobic digestion model, involving hydrogen and methane production, are described by a 12-dimensional nonlinear system of ordinary differential equations. The system's stability properties are analyzed, and numerical simulations illustrate the behavior of its trajectories for various initial conditions.

Mathematical Welfare Assessment Model for Lambs with Food Supplement Silimarin

N. Bozakova, V. Ivanov, S. Fidanova

In world practice, objective methods for assessing the welfare of farm animals are sought, through which the welfare of animals reared under different conditions can be compared. The aim of this study was to create a mathematical welfare assessing model of Lacaune lambs and, on this basis, to investigate the effect of a nutritional supplement Silymarin (2g/kg feed), for a welfare improving.
The complex method is based on the scientific concept of the Five freedoms that guxarantee animal welfare, given by the Animal Welfare Council of Great Britain (FAWC, 1995). Each of the Five freedoms was assessed on a 4-point scale, depending on its manifestation in lambs. The final mathematical assessment was calculated by summing the assessments of all five freedoms and relating them to the maximum possible welfare assessment -20, expressed in percentages.
The assessment of each of the freedoms was determined based on statistically significant changes between the control and experimental groups in the behaviour of the lambs, in the levels of corticosterone and serotonin in the blood and in some biochemical indicators. Using a mathematical model, the welfare of the control lambs was estimated at $AW_{control} = 50.50\%$. , and the welfare of the lambs with silymarin $-AW_{silymarin} = 75.00\%$ The hepatoprotector - silymarin contributed to the higher welfare of the experimental group, based on the better manifestation of the comfortable behaviour of the lambs, the decrease in the stress hormone levels - corticosterone and the improvement of liver enzymes in the experimental animals.

Comparative Analysis of Evolutionary Algorithms for Energy-Aware Production Scheduling

S.C. Burmeister, T.N. Rogalski, G. Schryen

The energy transition is driving rapid growth in renewable energy generation, creating the need to balance energy supply and demand with energy price awareness. One such approach for manufacturers to balance their energy demand with available energy is energy-aware production planning. Through energy-aware production planning, manufacturers can align their energy demand with dynamic grid conditions, supporting renewable energy integration while benefiting from lower prices and reduced emissions. Energy-aware production planning can be modeled as a multi-criteria scheduling problem, where the objectives extend beyond traditional metrics like makespan or required workers to also include minimizing energy costs and emissions. As production plans are frequently recalculated because of dynamic changes in the energy market and due to the NP-hard nature of this problem, evolutionary algorithms are widely used for energy-aware production scheduling. However, existing research focuses on individual algorithms, with limited comparisons between different approaches. In this study, we adapt NSGA-III, HypeE, and θ-DEA as memetic metaheuristics for energy-aware scheduling to minimize makespan, energy costs, emissions, and the number of workers, within a real-time energy market context. These adapted metaheuristics represent decomposition-based, indicator-based, and dominance-based approaches, respectively. In a comparative analysis, we explore differences in solution efficiency and quality across various scenarios which are based on benchmark instances from the literature and real-world energy market data. Additionally, we determine upper bounds of the gaps between objective values obtained with our memetic metaheuristics and optimal objective values using an exact solver, providing insights into their relative performance and approximation quality.

A Learning-accelerated Newton-Krylov-Schwarz Method and Applications

X.-C. Cai

We consider the numerical simulations of blood flows in the human artery with the incompressible Navier-Stokes equations, and the focus is on the situations when the artery is abnormal due to the existence of stenosis and/or aneurysm. The problem is discretized with a fully implicit finite element method and solved by a Newton-Krylov-Schwarz method which converges well when the solution is smooth but the convergence becomes unacceptably slow when abnormality of the artery is severe. For such difficult cases, we introduce an unsupervised learning based technique to reduce the stagnation and to speedup the convergence.

Robust Domain Decomposition Methods for High-Contrast Multiscale Problems on Irregular Domains

J. Calvo, J. Galvis

We propose a novel domain decomposition preconditioner for second-order elliptic partial differential equations, designed to efficiently handle coefficients with high-contrast and multiscale features. Unlike traditional approaches, our method is well-suited for irregular subdomains. The construction leverages partition of unity functions and carefully designed eigenvalue problems to enrich the standard coarse spaces. We establish that the condition number of the preconditioned systems is uniformly bounded, independent of the contrast in the coefficients. Additionally, we present selected numerical experiments that validate the robustness and effectiveness of the proposed preconditioner.

A Twofold Perturbed Saddle Point-Based Fully Mixed Finite Element Method for the Coupled Brinkman–Forchheimer/Darcy Problem

S. Carrasco, S. Caucao, G.N. Gatica

We introduce and analyze a new mixed finite element method for the stationary model arising from the coupling of the Brinkman–Forchheimer and Darcy equations. While the original unknowns are given by the velocities and pressures of the more and less permeable porous media, our approach is based on the introduction of the Brinkman–Forchheimer pseudostress as a further variable, which allows us to eliminate the respective pressure. Needless to say, the latter can be recovered later on by a postprocessing formula that depends only on the former. Next, aiming to perform a proper treatment of the transmission conditions, the traces on the interface, of both the Brinkman–Forchheimer velocity and the Darcy pressure, are also incorporated as auxiliary unknowns. Thus, the resulting fully-mixed variational formulation can be seen as a nonlinear perturbation of, in turn, a twofold perturbed saddle point operator equation. Additionally, the diagonal feature of some of the bilinear forms involved, facilitates the proof of their corresponding inf-sup conditions. Then, the fixed-point strategy arising from a linearization of the Forchheimer term, along with suitable abstract results exploiting the aforementioned structure, and the classical Banach theorem, are employed to prove the well-posedness of the continuous and discrete schemes. In particular, Raviart–Thomas and piecewise polynomial subspaces of the lowest degree for the domain unknowns, as well as continuous piecewise linear polynomials for the interface ones, constitute a feasible choice. Optimal error estimates and associated rates of convergence are established. Finally, several numerical results illustrating the good performance of the method and confirming the theoretical findings, are reported.

A Semi-Augmented Fully Mixed FEM for the Quasistatic Brinkman–Forchheimer/Darcy Model

S. Caucao, J. Esparza

We introduce and analyze a semi-augmented fully mixed formulation and a mixed finite element method for the coupled problem arising from the filtration of an incompressible fluid through a non-deformable saturated porous medium with heterogeneous permeability. The flow is governed by the Brinkman–Forchheimer and Darcy equations in the more and less permeable regions, respectively, with the corresponding transmission conditions defined by mass conservation and momentum continuity. We adopt dual-mixed formulations in both domains. Since the Brinkman–Forchheimer term requires the velocity to belong to a smaller function space than usual, we augment the variational formulation with appropriate Galerkin-type terms. Additionally, as the mass conservation condition becomes essential in the fully mixed formulation, it is imposed weakly by introducing the

trace of the Darcy pressure on the interface as a Lagrange multiplier. We establish the existence and uniqueness of a solution for the continuous weak formulation, as well as for a semidiscrete continuous-in-time formulation with nonmatching grids. These results are accompanied by stability bounds and error analysis with convergence rates. Finally, several numerical experiments are presented to validate the theoretical results and to illustrate the method's performance in applications involving flow through heterogeneous porous media.

Data-driven Finite Basis Method

Y. Choi

Traditional numerical methods for solving partial differential equations are widely employed in scientific discovery. However, as models are refined—such as through h-refinement or p-refinement—to better capture intricate system details, problem sizes can grow substantially due to the finer spatial and temporal discretization required. This expansion can easily reach exascale, significantly increasing computational costs. Furthermore, these refinements often introduce numerical instabilities, such as those stemming from CFL constraints and mesh distortions, which in turn limit time-step sizes and make long-duration simulations extremely challenging. Together, these factors create a major bottleneck in computational efficiency, impeding advancements in science and technology, particularly in scenarios that rely on critical decision-making.
To address these challenges, we propose integrating data-driven bases within a component-based reduced order model framework, enabling larger element sizes and scalable solutions for larger problems. This approach embodies the ideal machine learning paradigm: "train small, model big." By leveraging physics-driven identification of equations within the reduced space of each component, our method enables more robust extrapolation compared to purely data-driven approaches. In this talk, we will outline the general framework for component-based reduced order models and highlight substantial performance gains, including a 1000x speed-up in lattice-type structural design, a 1000x scale-up in nonlinear Navier–Stokes flow simulations over porous media, and extensions to nonlinear manifold reduced order models for time-dependent Burgers' equations.

Estimation of the High Wind Speeds over Bulgaria in the Projected Future Scenario-driven Climate

H. Chervenkov, K. Malcheva

Wind is an essential climate variable and a key meteorological parameter that significantly impacts the surface processes, hydrological cycle, air pollution, and wind energy production. High near-surface wind speeds, particularly wind gusts, can pose safety risks, both directly through structural damage and indirectly through sea waves and storm surges.

Therefore, it is essential to investigate the spatial distribution and frequency of high wind speeds in the projected future scenario-driven climate. Using the ECMWF's reanalysis ERA5 and a large ensemble of global circulation models from NEX- GDDP CMIP6, the study tries to quantitatively link daily mean wind speeds with daily maximum wind speeds for the territory of Bulgaria up to the end of the century, employing univariate linear regression. To evaluate the performance and accuracy of the regression model, three widely used metrics were selected: adjusted R-squared, regression standard error, and mean absolute percentage error. The capability of the regression model for predicting high wind speeds was evaluated using test data derived from the complete dataset. Also, the spatial and seasonal variations of the regression coefficients were investigated. The study reveals a substantial reduction in the number of days with strong winds in the last decades of the century compared to the near-past conditions under all four 'Tier 1' SSP scenarios. Our findings are probably a local reflection of the globally reported trend of decreasing wind speed over land, referred to as 'terrestrial stilling'.

Numerical Methods for Simulating Intrinsically Disordered Protein Regions

M. Chwastyk

In this talk, I will present refined approaches for describing interactions among intrinsically disordered regions in proteins at the single amino acid level. Accurately characterizing these interactions is essential for understanding the behavior of entire protein chains. Such precision is critical for elucidating processes like chain aggregation and the initiation of amyloid formation. These insights are particularly significant, as most neurodegenerative diseases – including Parkinson's, Alzheimer's, prion diseases, and tauopathies – are associated with protein aggregation, even though the aggregates themselves may not always be toxic. Additionally, understanding protein aggregation is important for studying membraneless organelles, which are proteinaceous liquid droplets formed by aggregates of intrinsically disordered proteins and often nucleic acids. During my talk, I will discuss numerical methods that are particularly useful for describing these phenomena.

High-performance Data Analytics for Analysis of Collective Trust Dynamics

D. Cvetković, S. Major, A. Tomašević, S. Maletić, M. Anđelković, A. Vranić, B. Stupovski, D. Vudragović, A. Alorić, A. Bogojević, M. Dankulov

Trust is a fundamental force that binds society together, yet the emergence and evolution of collective trust in social groups remain insufficiently understood. With over two billion active users engaging online, vast amounts of data provide an opportunity to analyze trust formation at a large scale. In this work, we integrate high-performance data analytics of empirical data to investigate how the structure of social networks influences trust dynamics. We aim to uncover key network properties that drive collective trust by leveraging complex network theory and novel topological methods. We apply this to data from three online platforms: Stack Exchange, Reddit, and Voat. Our results show that the early emergence of a stable and trustworthy core in StackExchange communities may be crucial for their sustainability. In the case of Reddit and Voat, we show that the structure of interactions between core and periphery users creates opportunities for users in the periphery to provide value to the community and increase their trustworthiness. We illustrate how different types of structures contribute to the dynamics of the number of active users and the role of collective trust in the sustainability of online social groups.

Minimally Intrusive Data-Driven Approximation of Schur Complement-based Coupling Operators for Heterogeneous Numerical Methods

A. de Castro, P. Bochev, P. Kuberry

Lagrange multiplier-based (LM) coupling approaches have been shown to be stable, accurate, and applicable to multiphysics problems coupled over an interface. For explicitly time-integrated coupled problems (IVR), the resulting Schur complement that is used to solve for the coupling traction forces is tractable but requires access to operators generally embedded deeply within the software modeling the subdomain. For implicitly time-integrated problems (IFR), the Schur complement involves inversion of stiffness matrices and is not computationally feasible. Through a data-driven discovery of coupling operators, we are able to loosen the requirement for access to multiple complex data structures and the resulting operator is more compact and less computationally expensive to evaluate than the full-order coupling operator.

With the rise in popularity of data-driven modeling techniques applied to subdomain problems, we make the assumption of the availability of full-resolution subdomain solution data on at least one subdomain and then leverage an idea by Carey et. al. from which to generate high-order approximations of traction forces for snapshots. We use the traction force snapshots to generate a reduced basis and then perform ordinary least squares operator regression to approximate the Schur complement system. The approach is minimally burdensome, requiring only Gramian matrices capturing a surface integral of solution trial and LM test functions over the interface.

We demonstrate the effectiveness of the technique with several numerical experiments and make comparison with respect to speed against Schwarz-based approaches and a full-order, Schur complement based approach.

A Quasi-Optimal Space-Time FEM With Local Mesh Refinements For Parabolic Problems

L. Diening, R. Stevenson, J. Storn

We present a space-time finite element method for the heat equation that computes quasi-optimal approximations with respect to natural norms while incorporating local mesh refinements in space-time. The discretized problem is solved with a conjugate gradient method with a (nearly) optimal preconditioner.

Efficient Monte Carlo Methods with Applications to Sensitivity Analysis

I. Dimov, R. Georgieva

Sensitivity analysis (SA) is a procedure for studying how sensitive are the output results of large-scale mathematical models to some uncertainties of the input data. The models are described as a system of partial differential equations. Often such systems contain a large number of input parameters. Obviously, it is important to know how sensitive is the solution to some uncontrolled variations or uncertainties in the input parameters of the model. Algorithms based on analysis of variances technique (ANOVA) for calculating numerical indicators of sensitivity and computationally efficient Monte Carlo integration techniques have recently been developed by the authors. They have been successfully applied to sensitivity studies of air pollution levels calculated by the Unified Danish Eulerian Model (UNI-DEM) with respect to several important input parameters. In this paper a comprehensive theoretical and experimental study of the Monte Carlo algorithm based on **"symmetrised shaking"** of Sobol sequences has been done. It has been proven that this algorithm has an optimal rate of convergence for functions with continuous and bounded second derivatives in terms of probability and mean square error. Extensive numerical experiments with Monte Carlo, quasi-Monte Carlo (QMC) and scrambled quasi-Monte Carlo algorithms based on Sobol sequences are performed to support the theoretical studies and to analyze applicability of the algorithms to various classes of problems. Various Monte Carlo algorithms for numerical integration have been applied to compute Sobol' global sensitivity indices. Among them a newly developed Monte Carlo algorithm based on Sobol' quasi-random points MCA-MSS has been applied. A comparison with sensitivity approaches implemented in SIMLAB software tool for sensitivity analysis has been done. The analysis and numerical results show advantages of MCA-MSS for relatively small sensitivity indices in terms of accuracy and efficiency.

A Web Based Decision Support Tool for Field Data Collection and Validation

N. Dobrinkova

Climate change and the socio-economic transformations have significantly increased the frequency and intensity of forest fires in European countries in the last 30 years. Traditional methods of monitoring and extinguishing forest fires often do not have the tools to predict the development of a given fire, which in some cases leads not only to economic losses, but also to human casualties. Bulgaria although its modest size is having breaking records burned areas and number of fires for the year of 2024 in comparison with the period 1970-2023, which is the official statistics of the county about wild land fire monitoring.

In such dynamic environmental changes decision support tools that can support data collection, data validation and optimization of the decision making processes are crucial. Meteorological conditions, detailed terrain information and vegetation types affected in cases of ignition point are the first and basic parameters, that the responsible authorities are looking for.

Thus in our article will be presented the architecture of a web-based tool which is available freely on-line for five test zones in the municipal areas of Kresna, Zlatograd, Svilengrad, Haskovo and Topolovgrad. The tool is part of the decision support process in the five municipalities and provide in real time data from local meteorological stations, represent in GIS layers information about the terrain, vegetation, water resources, evacuation safe spots and European Forest Fire Information System (EFFIS) warnings for the areas of the five municipalities.

A Sinc-function Based Numerical Method for the Dirichlet Problem with Fractional Laplacian

P. Dondl

This talk focuses on the numerical approximation of fractional differential operators and their applications in the corresponding partial differential equations.

As a model problem, we consider the approximation of the integral fractional Laplacian $(-\Delta)^s$. We approximate it using a basis formed by dilated and shifted tensor products of sinc functions. This approach is motivated by the representation of the fractional Laplacian as a Fourier multiplier $|\omega|^{2s}$ and the simple structure of the sinc basis functions in the Fourier domain, where they correspond to indicator functions of hypercubes in $\mathbf{R}^d$. These two ingredients enable the development of efficient numerical schemes for computing discrete operators in the sinc basis and applying them via efficient discrete convolution. The linear systems resulting from the discretization of the corresponding PDEs are solved using iterative methods. This approach is computationally viable because the discrete convolution can be performed efficiently using Fourier techniques. To accelerate convergence, we employ appropriately constructed periodic operators as preconditioners.

To ensure that the solutions obtained via this discretization converge to the analytical solutions, we reformulate the sinc-collocation method as an equivalent Galerkin method. Leveraging this formulation, we use abstract error estimates to prove convergence rates comparable to those of finite element discretizations with the same spacing.
We substantiate the theoretical analysis with extensive numerical experiments in up to $d = 3$ spatial dimensions. These experiments include the numerical solution of the Dirichlet problem for the fractional Laplacian on various domains and demonstrate its applicability across multiple scenarios.

Preconditioning Techniques for Fully Implicit Runge–Kutta Methods

I. Dravins

Fully implicit Runge–Kutta methods offer the possibility to use high-order-accurate time discretization with desirable stability properties. For general implicit Runge–Kutta methods all stages are coupled leading to a potentially costly and involved solution procedure which has been a major barrier to their widespread use.
We present a stage-parallel block preconditioner for the class of L-stable Radau IIA Runge–Kutta methods. The preconditioner exploits a property of the coefficient matrices to construct a block lower-triangular preconditioner. During the application of the preconditioner, a basis change can be applied to obtain a block-diagonal form, in this way allowing us to decouple the stages when solving for the blocks. In the linear case this basis change can be applied directly – for non-linear equations further approximations are needed to achieve this decoupling.
For the linear case, we discuss the analysis of the preconditioned matrices which are non-symmetric and in tensor form. We give eigenvalue bounds for a range of stages under symmetric positive definite assumptions. Furthermore, we discuss what can be shown for the general non-symmetric case.
We illustrate the performance by numerical examples, including also applications to non-linear problems. The parallel behavior is demonstrated, comparing space-parallel but serial in stages against fully stage-parallel implementations on HPC platforms. Finally, we discuss mixed precision aspects and implementations utilizing GPUs.

Stage-Parallel Runge-Kutta Methods via Low-Rank Matrix Equation Corrections

F. Durastante, M. Mazza

Implicit Runge-Kutta (IRK) methods are highly effective for solving stiff ordinary differential equations (ODEs)

$$\begin{aligned} &My'(t) = f(y(t), t), \quad t \in [0, T], \\ &y(0) = y_0. \end{aligned}$$

However, their usage can be computationally expensive for large-scale problems due to the need to solve coupled algebraic equations at each step. This study improves IRK efficiency by leveraging parallelism to decouple stage computations and reduce communication overhead. In the linear case, the generic RK method takes the form

$$\begin{aligned} &My'(t) = -Ly(t) + \hat{f}(t), \\ &y(0) = y_0, \end{aligned} \qquad M, L \in R^{N \times N},$$

for which the computational expensive step is given by the computation of the stages K by

$$MK = -Ly_n 1_s^\top - hLKA^\top + F.$$

If the stage matrix A was diagonalizable as $A = X\Lambda X^{-1}$, this could be solved by doing

$$\begin{aligned} &r = -(X^{-1}1_s \otimes L)y_n + (X^{-1} \otimes I)\operatorname{vec}(F), \\ &(I_s \otimes M + h\Lambda \otimes L)\, z = r, \\ &\operatorname{vec}(K) = (X \otimes I)\, z. \end{aligned}$$

This is not the case in general. Nevertheless, for three well-known IRK families—symmetric methods, collocation methods, and Hamiltonian Boundary Value Methods—we write A as the sum of a diagonalizable plus a low-rank matrix. With this we devise a strategy using the parallel block-diagonal solution in the previous equation followed by a sequential matrix-equation solution to advance the method. We illustrate the idea with several numerical examples and discuss the extension to the more general nonlinear setting.

Multiscale Finite Element Methods and Relation to Multicontinuum Homogenization

Y. Efendiev

I will start with past joint multiscale research with Raytcho Lazarov and discuss the evolution of these methods and some new approaches in multicontinuum homogenization.

A Fixed-Point Iteration for Nonlinear Time-Periodic Parabolic Problems

H. Egger, A. Schafelner

We present a fixed-point iteration for the solution of nonlinear parabolic time-periodic evolution equations. Such equations arise, for instance, in electrical engineering when simulating the magnetic field inside an electrical motor or transformer. We show the existence of a unique solution of the fixed-point equation that is equivalent to the solution of the evolution equation. The proof is constructive and thus also yields a numerical scheme. In order to speed up convergence of the method, we will explore different options for preconditioning and examine their efficiency and parallel performance. In the end, we present numerical experiments where we apply the method to magnetic field simulations inside a transformer.

Goal-Oriented Adaptive Space-Time Finite Element Methods for the Parabolic p-Laplace Equation

B. Endtmayer, U. Langer, A. Schafelner

In this presentation, we will derive goal-oriented error estimations for the parabolic p-Laplace problem. The approach employs a fully unstructured space-time grid, offering flexibility and adaptability. For the error estimation and the adaptivity the dual weighted residual method is used. Under a saturation assumption, the method is proven to be both efficient and reliable. Lastly, the theoretical findings are supported by numerical experiments.

FEM-BEM Coupling in Fractional Diffusion

M. Faustmann, A. Rieder

In this talk, we consider fractional differential equations posed on the full space $\mathbb{R}^d$. A distinct advantage of full-space formulations for fractional PDEs is that all common definitions of non-integer powers of differential operators are equivalent, which is not true for formulations on bounded domains.
In order to treat the full-space problem numerically, serveral reformulations have to be made. Starting with the well-known Caffarelli-Silvestre extension to $\mathbb{R}^d \times \mathbb{R}^+$, we truncate the extension problem in the extended variable only to $\mathbb{R}^d \times (0, \mathcal{Y})$ for some $\mathcal{Y} > 0$. Then, a diagonalization procedure, similar to the case of the spectral fractional Laplacian on bounded domains, can be employed that leads to a sequence of scalar Helmholtz-type problems, which are discretized with a symmetric coupling of finite elements and

boundary elements. Combined with a hp-FEM discretization in the extended variable, this gives a fully computable approximation with reasonable computational effort.
For the mentioned reformulations, we show well-posedness in certain exotic Hilbert spaces. Using purely variational techniques, we derive an algebraic rate of decay of the solution of the truncated problem to the full-space solution as $\mathcal{Y} \to \infty$ as well as estimates of weighted analytic type for higher order derivatives of the truncated extension problem. These decay and regularity estimates can be used to derive a-priori estimates for the error between the exact full-space solution and an approximation based on our approach using a coupling of finite elements and boundary elements.

R3MG: R-tree Based Agglomeration of Polytopal Grids with Applications to Multilevel Methods

M. Feder, A. Cangiani, L. Heltai, P.C. Africa

Agglomeration strategies are a key ingredient in polytopal methods for PDEs as they are used to generate (hierarchies of) computational grids from an initial grid. We present a novel approach to perform agglomeration of polygonal and polyhedral grids based on spatial indices. We show how the construction of the R-tree spatial database of an arbitrary fine grid offers a natural and efficient agglomeration strategy. It has been validated against traditional approaches showing superior or comparable results at a fraction of the computational cost. Our process is fully automated, robust, and automatically produces a balanced and nested hierarchy of agglomerates which allows geometric multigrid methods to be applied also to those cases where a hierarchy of grids is not directly available. We will discuss its memory-distributed implementation, which builds on top of the `deal.II` Finite Element library, and show the effectiveness of our approach with examples in the context of non-trivial three-dimensional geometries and the design of geometric multigrid preconditioners. Finally, we apply our methodology to construct a geometric multigrid preconditioner for the Discontinuous Galerkin discretization of the monodomain problem, one of the central models in cardiac electrophysiology.

Dynamic Programming Techniques for Orbital Transfer of Low Earth Orbit Satellites

R. Ferretti, G. Villani

We present an application of the optimal control theory to orbital transfer of Low Earth Orbit satellites from the pre-operating towards the operating orbit. The optimal control problem is treated with Dynamic Programming techniques which require solving the Hamilton–Jacobi–Bellman equation on a suitable state space, with the reconstruction of the optimal controls made in the form of a static feedback.

In order to validate the numerical scheme without the complexity of the full model, a first study sets the problem in planar form, thus working in a four-dimensional state space. We study various techniques to speed up the computation, and assess the accuracy of the numerical solution. In a second phase, the complete 3-D problem is tackled.
This project is born from the attempt of evaluating and applying the (relatively unusual) optimal control techniques based on Dynamic Program- ming as a complementary approach to the well-known indirect methods, like Pontryagin or Lawden. This goes in the direction of implementing a feedback strategy which might be part of an on-board controller. In particular, the final aim is to treat the case of low thrust engines from real use cases, in the full 3-D problem.

Advances in Multi-physics and Multi-domain Simulations of Coupled Poromechanics

M. Ferronato, A. Franceschini, D. Moretto

It is very well-known that coupled poromechanical simulations play a crucial role for a proper management of underground resources, involving multiple physical processes, such as fluid flow, poromechanics, fault activation, thermal flow, and chemical reactions, that can take place simultaneously with multiple time and space scales. The present communication focusses on the development of GReS, a novel open-source modular platform specifically designed with the aim at contributing to the design and testing of numerical algorithms for fully coupled multi-physics multi-domain poromechanical applications. The idea is to partition the overall computational domain into possibly non-conforming subdomains where different physics and discretization schemes can be used. The code is based on a high-level programming platform (MATLAB) that should lower the entry barrier for new users and developers, as well as the effort for implementing and testing innovative numerical algorithms. Moreover, the modular structure of the code encourages contributions from different developers at variable levels, from the implementation of new physics and discretization schemes to specific algorithms to accelerate the linear and non-linear solver. Despite being primarily conceived as a prototyping platform, GReS wraps low-level advanced linear algebra packages to combine simplicity with fair efficiency. In the present communication, we will introduce the GReS concept and its current development state, including advances to the mortar algorithm used to transfer the information among non-conforming subdomains with independent meshes. Basic benchmarks will be presented to show the current code potentials, along with the projects for future developments.

Generalized Net for Evacuation of Cows During an Earthquake

S. Fidanova, V. Ivanov, N. Bozakova, L. Kirilov

Natural disasters can cause great damage to agriculture and especially livestock farming. It plays an important role in the economies of countries. It is especially important for feeding the population. An earthquake can cause major damage to farm buildings and from there to losses. Animals are very sensitive to earthquakes. Such an event could cause panic among them. Numerous animals in panic can cause major property damage. They also pose a danger to humans. It is necessary to establish a good organization for the evacuation of animals in advance. To this end, the behavior and reaction of animals in various disaster situations must be studied. The evacuation model should include the method of evacuation for the relevant type of animal, evacuation logistics, and shelter location. Evacuation logistics include assessment of damage and the need for evacuation, evacuation costs, evacuation losses, available road network for evacuation, need and availability of evacuation transport, necessary personnel resources for evacuation. In this work, we have proposed a generalized network-based model for earthquake evacuation. The model can be used to optimize evacuation and reduce losses to farmers and potential damage that cows can cause. The model can also serve authorities to define various policies to support and protect livestock farming.

Space-Time Modeling, Discretization, And Goal-Oriented Error Estimation Of Coupled Problems

H. Fischer, V. Kosin, J. Roth, J.P. Thiele, T. Wick

In this presentation, we discuss recent progress in space-time numerical modeling of coupled problems. Under the terminology coupled problems, we understand nonstationary, nonlinear, coupled PDE systems up to coupled variational inequalities systems (CVIS). Having space-time models at hand, we consider goal-oriented a posteriori error control and adaptivity with the dual-weighted residual method for incompressible flow (Navier-Stokes equations), fluid-structure interaction, and phase-field fracture. Therein, a linear backward-in-time adjoint problem must be designed to obtain sensitivity measures with respect to the goal functional(s). Error localization is done with a partition-of-unity approach proposed by Richter and Wick (2015) and recently extended to a space-time partition-of-unity by Endtmayer, Langer, Schafelner (2024), Thiele, Wick (2024), and Endtmayer, Langer, Richter, Schafelner, Wick (2024). If time permits, furthermore, we briefly give insights to space-time modeling of multirate schemes and goal-oriented error-controlled incremental proper orthogonal decomposition model order reduction. These two concepts are applied to the Biot system in porous media by considering the Mandel benchmark. All algorithms are substantiated with computational convergence studies and computational cost analyses.

Well-Posedness of Fully Discrete Fractional Elasto-Plasticity

M. Feischl, D. Niederkofler, B. Wohlmuth

We consider a fractional plasticity model based on linear isotropic and kinematic hardening as well as a standard von-Mises yield function, where the flow rule is replaced by a Riesz-Caputo fractional derivative. The resulting mathematical model is typically non-local and non-smooth and even basic questions such as how to design well-posed discretizations are open. We propose new numerical algorithms based on the well-known radial return mapping, which exploit that the kernel of the Riesz-Caputo derivative is finitely supported.
We investigate explicit and implicit discretizations of the model and show the well-posedness of the explicit-in-time discretization, which employs standard finite elements to resolve the space. Numerical results in two and three dimensions illustrate the performance of the algorithm and furthermore clearly show the distinct modeling behavior of the fractional model when compared to classical non-fractional approaches.

Depth Averaged Material Point Models for Landslide Simulations

L. Formaggia, C. de Falco, M. Fois

Landslides are among the most dangerous natural disasters, with their unpredictability and potential for catastrophic human and economic losses exacerbated by climate change. Continuous monitoring and precise modeling of landslide-prone areas are crucial for effective risk management and mitigation. After a general presentation of the problem, this talk illustrates the results obtained by numerical approach based on a depth averaged material particle model (MPM).
The method has been chosen for its efficiency and parallel properties, enabling fast computation in view of its use for uncertainty quantification and scenario analysis. The simulation results are rigorously tested against benchmarks and applied to a real-world scenario with topography reconstructed from satelite data.
We make some consideration of parallel efficiency and comparisons with a different, mesh-based, approach are also discussed.

The research was partially supported by the *Accordo Attuativo ASI-POLIMI "Attività di Ricerca e Innovazione" n. 2018-5-HH.0.* and by the Italian Research Center on High-Performance Computing, Big Data and Quantum Computing (ICSC), European Union - Next Generation EU.

References

[1] Fois, M., Gatti, F., de Falco, C., Formaggia, L. (2024). *A comparative analysis of mesh-based and particle-based numerical methods for landslide run-out simulations*, MOX-Report No. 103/2024

[2] Fois, M., de Falco, C., Formaggia, L. (2024) *A semi-conservative depth-averaged material point method for fast flow-like landslides and mudflows*, Communications in Nonlinear Science and Numerical Simulation, 138, 108202

Space-Time FEM-BEM Couplings for Parabolic Transmission Problems

T. Führer, G. Gantner, M. Karkulik

In this talk, we discuss the first provably stable couplings of space-time finite and boundary element methods (FEM-BEM) for the numerical solution of parabolic transmission problems on the full space and a finite time interval. The couplings are based on a recent space-time first-order system least-squares (FOSLS) method in the interior and space-time BEM in the exterior. In particular, we demonstrate coercivity of the couplings under certain restrictions and validate our theoretical findings by numerical experiments.

Influence of Grid Resolution on Ozone (O_3) Process Analysis Evaluation

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

Air pollution is of big concern in many countries, despite different measures taken by the local authorities. The meteorological and chemical-transport models capabilities depend on many factors, as the descriptions of their physics, dynamics, chemical transformations and spatial-temporal grid resolutions. The implications emerging from these properties are important for the robust interpretation of the model results, which in turn influences the final decisions concerning the air quality in specific city, country, or region as a whole. The current study concerning the processes determining the Ozone (O_3). The O_3 is important not only in troposphere, but also in the stratosphere. The stratospheric Ozone in the Earth's atmosphere is formed under the influence of solar radiation and is distributed under the influence of atmospheric dynamics. Stratospheric ozone forms a protective layer that protects the Earth's biosphere from the harmful effects of ultraviolet solar radiation in the 280-315 nm range. Variations in this ozone layer are caused by seasonal changes in atmospheric dynamics, particularly stratospheric warming. The current study is focused only the surface O_3 in Bulgaria, according to previous results show that this pollutant are among the ones that are responsible for the most frequent episodes of air quality deterioration in both urban and rural sites. The main goal of that research is to display the effect of grid size of the emissions and process description on the different mechanisms responsible for the concentration of Ozone (O_3) over Bulgaria. For that purpose, a system of three models was used: meteorological, emission and chemical-transport model (WRF, SMOKE and CMAQ). The numerical experiments for different cases indicated the lead impact of the grid resolution on the concentrations and the dynamical and chemical processes contribution on the concentrations. The presented results in the paper display that, for simulation of the atmospheric composition, the grid and the source description resolution play a significant role.

Hierarchical Super-Localized Orthogonal Decomposition Method

J.C. Garay, H. Mohr, D. Peterseim, C. Zimmer

We present the construction of a sparse-compressed operator that approximates the solution operator of elliptic partial differential equations (PDE) with rough coefficients. To derive the compressed operator, we construct a hierarchical basis of an approximate solution space, with superlocalized basis functions that are quasi-orthogonal across hierarchy levels with respect to the inner product induced by the energy norm. The superlocalization is achieved through a novel variant of the Super-Localized Orthogonal Decomposition method that is built upon corrections of basis functions arising from the Localized Orthogonal Decomposition method. The hierarchical basis not only induces a sparse compression of the solution space but also enables an orthogonal multiresolution decomposition of the approximate solution operator, decoupling scales and solution contributions of each level of the hierarchy. With this decomposition, the solution of the PDE reduces to the solution of a set of independent linear systems (one system per level) with mesh-independent condition numbers that can be computed simultaneously. We present an accuracy study of the compressed solution operator as well as numerical results illustrating our theoretical findings and beyond, revealing that desired optimal error rates with well-behaved superlocalized basis functions can still be attained even in the challenging case of coefficients with high-contrast channels.

Mixed Finite Element Methods for the Coupled Biot and Poisson–Nernst–Planck Equations

G.N. Gatica, C. Inzunza, R. Ruiz-Baier

We propose mixed finite element methods for the coupled Biot poroelasticity and Poisson–Nernst–Planck equations (modeling ion transport in deformable porous media). For the poroelasticity, we consider a primal-mixed, four-field formulation in terms of the solid displacement, the fluid pressure, the Darcy flux, and the total pressure. In turn, the Poisson–Nernst–Planck equations are formulated in terms of the electrostatic potential, the electric field, the ionized particle concentrations, their gradients, and the total ionic fluxes. The weak formulation, posed in Banach spaces, exhibits the structure of a perturbed block-diagonal operator consisting of perturbed and generalized saddle-point problems for the Biot equations, a generalized saddle-point system for the Poisson equations, and a perturbed twofold saddle-point problem for the Nernst–Planck equations. One of the main novelties here is the well-posedness analysis, hinging on the Banach fixed-point theorem along with small data assumptions, the Babuška–Brezzi theory in Banach spaces, and a slight variant of recent abstract results for perturbed saddle-point problems, again in Banach spaces. The associated Galerkin scheme is addressed similarly, employing the Banach fixed-point theorem to yield discrete well-posedness. A priori error estimates are derived, and simple numerical examples validate the theoretical error bounds, and illustrate the performance of the proposed schemes.

Development and Application of Drawdown Measure in the Optimization of Precious Metals Portfolio

S. Georgiev, B. Idirizov

The study investigates the application of the Conditional Drawdown-at-Risk (CDaR) measure in optimizing precious metals portfolios, focusing on silver and gold. Conditional Drawdown-at-Risk, incorporating maximum and average drawdowns as limiting cases, has proven to effectively capture risk dynamics under market uncertainty. A methodological approach is utilized to account for drawdowns, significantly reducing the influence of inflation over time on the integrity and precision of the measure's valuation. By mitigating reduced inflation effects, the method enhances portfolio resilience and performance. It is utilized to effectively solve a practical portfolio optimization problem. Results demonstrate CDaR's utility in managing and minimizing downside risks. The Conditional Drawdown-at-Risk function is based on the principles of the Conditional Value-at-Risk measure. The integration of CDaR in portfolio management emphasizes its potential as a superior risk metric compared to traditional measures, providing critical insights for investors seeking stability in precious metals investment strategies.

Numerical Boundary Control of Semilinear Hyperbolic Systems

S. Gerster, A. Sikstel, F. Nagel, G. Visconti

Physical systems such as gas networks are usually operated in a state of equilibrium and one is interested in stable systems, where small perturbations are damped over time. This talk is devoted to the design of boundary controls of systems that are described by hyperbolic balance laws. An underlying tool for the study of these problems are Lyapunov functions that yield upper bounds on the deviation from steady states in suitable norms. Furthermore, numerical approaches and limits of stabilizability are discussed.

Higher-order Finite Element Methods for the Fractional Laplacian

H. Gimperlein

Diffusion processes beyond Brownian motion have recently attracted significant interest from different communities in mathematics, the physical and biological sciences. They are described by partial differential equations involving nonlocal operators with singular non-integrable kernels, such as the integral fractional Laplacian. This talk surveys results, in particular, obtained in collaboration with E. P. Stephan, J. Stocek and C. Urzua-Torres, on asymptotic expansions of the solution, the resulting a priori error estimates for h, p and hp-versions, as well as the operator preconditioning.

Power Contractivity for RAS-Imp and RAS-PML for the Helmholtz Equation

S. Gong

We consider two variants of restricted overlapping Schwarz methods for the Helmholtz equation. The first method, known as RAS-Imp, incorporates impedance boundary condition to formulate the local problems. The second method, RAS-PML, employs local perfectly matched layers (PML). These methods combine the local solutions additively with a partition of unity. We have shown that RAS-Imp has power contractivity for strip domain decompositions. More recently, we shown that RAS-PML has super-algebraic convergence with respective to wavenumber after a specified number of iterations. In this talk we review these results and then investigate their sharpness using numerical experiments. We also investigate situations not covered by the theory. In particular, the theory needs the overlap of the domains or the PML widths to be independent of k. We present numerical experiments where this distances decrease with k. This is a joint work with Jeffrey Galkowski, Ivan Graham, David Lafontaine and Euan Spence.

Ultraweak DPG Formulations, Optimal Norms, and Applications

J. Gopalakrishnan

We report on some new results contained in a forthcoming review of the Discontinuous Petrov Galerkin (DPG) methods (to appear in Acta Numerica). One of the new results gives norms on the test and trial spaces of any ultraweak DPG formulation that make the bilinear form act like a duality pairing. The significance of this property is that in such norms, both the continuity and inf-sup constants are one. Relating the norm to Peetre's K-functional, equivalences that help one understand the norm better are presented. The interest in such results stem from potential parameter robustness properties derivable from it. Emerging applications to parameter robustness that are useful in learning parameter-to-solution maps will be discussed.

Speeding up an Unsteady Flow Simulation by Adaptive BDDC and Krylov Subspace Recycling

M. Hanek, J. Papež, <u>J. Šístek</u>

Means of acceleration of iterative methods for sequences of linear systems have been extensively studied in literature. A widely used approach is recycling the subspace within a Krylov method combined with deflation. Another natural approach is based on improving the preconditioner. In domain decomposition methods, adaptive selection of coarse space is the state of the art leading to powerful preconditioners.

We compare these two approaches and study their combination for unsteady incompressible flow problems governed by the Navier-Stokes equations. These are solved by the pressure-correction scheme in connection with the finite element method. This approach leads to sequences of linear systems over the time steps.
Our particular interest is the Poisson problem of pressure. Results for the problem of flow behind the sphere for Reynolds numbers 100 and 300 are presented. We demonstrate that by using these approaches we are able to save about one half of the computational time.

Numerically Efficient Approximations of Fractional Powers of SPD Matrices, Inheriting the Key Properties of the Operator

S. Harizanov

Fractional diffusion has many applications in science and engineering as it models non-local processes and phenomena. However, numerically solving such problems involves systems of linear algebraic equations with dense matrices. The Best Uniform Rational Approximation (BURA) and related methods have been developed in order to compute an approximation of the inverse $\mathbb{A}^{-\alpha}$ of a symmetric positive definite matrix $\mathbb{A}$ via an approximation of the scalar function $t^\alpha, \alpha \in (0,1), t \in [0,1]$. Thus, the solution a system of linear algebraic equations $\mathbb{A}^\alpha \mathbf{u} = \mathbf{f}$ can be computed approximately via computing several auxiliary systems with as sparse matrices as $\mathbb{A}$.
There are several applicable approaches for solving the numerical problem, when $\alpha \in (0,1)$. Unfortunately, most of them heavily rely on the parameter interval and do not work for other alphas. Even though the BURA method does work in the generalized setting, its direct application may not preserve the SPD key property of the approximant. In this talk, we present indirect BURA alternatives, based on a superposition of BURA elements for $\alpha_i \in (0,1)$, that are both numerically efficient and inherit the properties of the original operator. We provide a theoretical, as well as an experimental, analysis on the approximation errors of those operators.

Iterative Methods For Large-Scale Elastic Graphs

M. Hauck, A. Målqvist, A. Rupp

This talk deals with the numerical solution of Timoshenko beam network models, i.e., Timoshenko beam equations at each edge of the network, coupled at the nodes of the network by rigid joint conditions. A prominent application of such models is the simulation of fiber-based materials such as paper or cardboard. Similar models can also be applied to describe flow in porous media as well as poromechanics. Through hybridization, we can reformulate the problem equivalently as a symmetric positive definite system of linear equations posed at the nodes of the network. This is possible because the nodes to which the beam equations are coupled are zero-dimensional objects. To discretize the beam network model, we apply a hybridizable discontinuous Galerkin method that can achieve arbitrary orders of convergence under mesh refinement without increasing the size of the global system matrix. As a preconditioner for the typically very poorly conditioned global system matrix, we employ a two-level overlapping additive Schwarz method. We prove uniform convergence of the corresponding preconditioned conjugate gradient method under appropriate connectivity assumptions on the network. Numerical experiments demonstrate the practical performance of the method.

Porous Media Free-Flow Coupling - From REV to Pore Scale and Back

R. Helmig, M. Schneider, H. Wu, M. Veyskarami, I. Yotov

Flow and transport processes in domains composed of a porous medium and an adjacent free-flow region appear in a wide range of industrial, bio-medical and environmental applications. Industrial applications range from flow in fuel cells to drying processes; possible bio-medical applications include the interplay of distribution processes in blood vessels and in the surrounding tissue. Applications in environmental systems include infiltration of overland flow during rainfall, groundwater contamination due to infiltrating pollutants and evaporation from soil.
One of the key challenges for coupled free flow and porous-medium flow arises from the fact that the overall effective behaviour depends strongly on interface processes that occur on small spatial scales (pore scale), although the overall system of interest is often too large to resolve these processes explicitly in detail. REV-scale models are usually not able to capture all the relevant physical processes for such coupled systems. For the accurate description of interface phenomena, it is therefore necessary to develop model concepts that combine information gained through pore-scale and REV-scale models

Vertex Centered Control Volume Mimetic Finite Difference Methods

R. Helmig, M. Schneider, I. Yotov

We develop a new class of vertex-centered control-volume mimetic finite difference methods on polytopal meshes for second order elliptic equations. The schemes are based on a mixed velocity-pressure formulation. The pressure is constant on dual mesh control-volumes constructed around the primary mesh vertices. The normal velocity is constant on the faces of the control-volumes, resulting in local mass conservation over the control-volumes. We consider both symmetric velocity integration rules constructed over the control-volumes, as well as non-symmetric quadrature rules constructed over sub-volumes obtained by the intersection of primary and dual elements. The latter choice allows for

explicit gradient construction and local multipoint flux elimination within the primary elements, resulting in a positive definite vertex-centered pressure system. On simplicial, quadrilateral or hexahedral meshes, these local flux methods are closely related, and in some cases equivalent, to the classical vertex-centered control-volume finite element methods based on piecewise polynomial finite element basis functions for the pressure. The mimetic finite difference framework is utilized to analyze the well posedness and accuracy of the proposed methods. We establish first order convergence for the pressure and the velocity in the discrete mimetic norms, as well as second order pressure superconvergence in the case of symmetric quadrature rules. A series of numerical experiments illustrates the convergence properties of the methods on problems with varying degree of anisotropy, heterogeneity, and grid complexity in two and three dimensions.

On Modeling and Simulation of Heat and Mass Transfer with Phase Changes on the Examples of Solidification of Metals and Near Infrared Drying of Lithium-Ion Battery's Electrode

O. Iliev

In 70s and 80s of the last century Raytcho Lazarov was leading in the Institute of Mathematics, BAS, a group on modeling and simulation of heat and mass transfer processes in the presence of phase change. The specific topic was solidification of metals and alloys, and the research and development was carried out as part of the collaboration between the Institute of Mathematics the Institute of Metal Science of BAS.

In the first part of this talk some of the results obtained at that time under the leadership of Raytcho will be recalled. In the second part of the talk another heat and mass transfer problem with phase change will be discussed, namely, drying of LIB electrode during its production.

Currently, convective drying is used by industry in the vast majority of battery electrode manufacturing processes. However, it is characterized by very high energy consumption and there are also limitations on the production speed. There is a demand for more efficient drying processes. Among the several technologies which are studied currently, the most promising and closest to the industrial standards is the near infrared radiation, NIR. There are a great number of experimental and numerical papers on convective drying, but NIR is still not widely studied. In this paper, we present an experimental and numerical study of electrode drying, including those with high-intensity NIR. We report several findings: (i) no vertical temperature gradient is observed in the carried experiments; (ii) NIR enables fast drying with good adhesion; (iii) no capillary limitations are observed in NIR drying of thin electrodes; (iv) presented comparison between the experimental and numerical results, shows that the model used correctly represents the experiment; (v) we elaborate on how NIR is heating the slurry volumetrically, in contrast to the surface heating in the convective drying.

Differential Inclusions and Quasi-Lyapunov Functions

M. Ivanov, M. Krastanov, N. Ribarska

We study the existence of solutions of differential inclusions of the form

$$\dot{x} \in F(x),\, x(0) = x_0,$$

where $x_0 \in \mathbb{R}^n$ and $F : \mathbb{R}^n \rightrightarrows \mathbb{R}^n$ is a multi-valued mapping with nonempty values.
A sufficient condition for the existence of a solution of a differential inclusion with uniformly bounded right-hand side with nonempty closed (possibly nonconvex) values is obtained. We propose a way to cope with the so-called "bad points". We assume the existence of a function that keeps the ε-solutions of the inclusion starting from "good points" away from the set of "bad points". In this way, we prove that it is possible to construct a solution starting from a point on the boundary of the set of "bad points". The function in question (called quasi-Lyapunov function) is assumed to be piecewise smooth.
We obtain an Olech type result as a corollary and we show that the main result is applicable to an inclusion which originates from the optimal feedback for the Fuller's problem from the optimal control theory. We construct a quasi-Lyapunov function in this example which is semi-algebraic.

Probing Convolutional NN Architectures for Binding Affinity Assessment in Computational Drug Design

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

Protein-protein and protein-peptide interactions (PPIs) are central to numerous critical cellular processes. A thorough understanding of these interactions is vital for elucidating cellular mechanisms and plays a pivotal role in the development of drugs designed to regulate them.
The investigation of PPIs is inherently challenging, as traditional experimental methods are both time-consuming and resource-intensive. To address these challenges, machine learning (ML) and artificial intelligence (AI) models have been employed to identify binding sites on target proteins and estimate ligand binding affinity, often utilizing scoring functions. Among these, convolutional neural networks (CNNs) have emerged as the most reliable and widely used frameworks.
A more targeted strategy for studying PPIs involves determining the binding energy of protein-peptide complexes. While numerous ML models exist for predicting various attributes of protein complexes, none are currently recognized as dependable for accurately estimating the binding energy of interacting biomolecules.
In this work, we propose a novel approach that digitizes the three-dimensional structural data of protein-protein and protein-peptide complexes. Additionally, we introduce a minimal convolutional network architecture that demonstrates significant potential for accurately predicting the binding energy of these molecular complexes.

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Identification of Vulnerable Population Groups in Disasters

V. Ivanov, S. Fidanova, N. Bozakova, G. Rusev, L. Kirilov

Natural and anthropogenic disasters have happened ever since the dawn of time and human history. Thousands of people have lost their lives or have suffered different health impairments due to disasters like earthquakes, floods, volcanic eruptions, military conflicts, acts of terrorism, chemical and nuclear accidents, etc. Nevertheless, some social groups are particularly vulnerable in such extreme situations. In such groups, the number of casualties and victims is noticeably and disproportionally bigger in comparison with the total number of the population affected. In fact, it seems that the social status differences are most clearly visible in disaster situations.
The purpose of this research is to identify such vulnerable groups in our society, with the aim of organizing advance preparation actions with regard to improving prevention and minimizing the aftermath, the number of victims and the effects of natural or manmade disasters among such groups. The main challenge when planning ways of managing disasters is to properly identify the most vulnerable groups, the proper assessment of social inequalities and providing protection to vulnerable members of a society by organizing priority evacuation of the most vulnerable groups and giving them help according their needs.

Oscillatory Controls that Generate Motion in Distinguished Directions

M. Kawski

We consider the path planning problem for nonholonomic control systems. For systems with planar controls we present innovations that dramatically improve the classic algorithm presented by Chitour, Jean and Long in their 2013 article *A global steering method for nonholonomic systems.*
The starting point is an exponential product expansion for the flow in terms of Hall bases for the free Lie algebra and their dual bases of iterated integral functionals.
A perfect solution would be a set of simple controls that selectively only activate motion in the direction of one basic Hall element (iterated Lie bracket of the vector fields defining the system). This corresponds to all but one of the dual iterated integral coefficients vanishing on that control input. In the case of the free nilpotent system in infinite dimensions this may be even impossible without inventing generalized controls. In finite dimensions a good practical sets of control inputs may not be diagonal, but only lower triangular on the set of iterated integral functionals. In practice, as demonstrated in

that classic article, one henceforth performs successive motions to correct the side effects caused by the imperfect sets of controls. We also analyze the effort needed (consider this as the energy needed) to move a fixed amount into any direction, and the additional energy needed for the corrections. This is of particular interest as the dimensions of the system increase.
We demonstrate that in the case of planar controls one can generate the desired compound motions with frequencies that are orders of magnitude lower than those in the classic paper. Key innovations include symmetries acting on the control inputs to overcome combinatorial constraints from mismatches of the numbers of available frequencies and the number of directions.

The Effect of Hydrogen on Interfacial Plasticity in Lath Martensite Steel

I.H. Katzarov

The present study aims to extend the current understanding of the effect of hydrogen on nano-scale deformation mechanisms in lath martensite structures. The presence of hydrogen deteriorates the mechanical properties of lath martensitic steels, leading to reduced ductility and strength. A lath martensite grain is divided into packets comprising blocks and sub-blocks, which are constructed from parallel laths of martensite. It is assumed that lath martensite is particularly susceptible to hydrogen embrittlement due to the high density of lath/block boundaries. Experimental observations reveal strain localization at block and packet boundaries in the form of interface plasticity. However, the nano-scale mechanisms responsible for the observed interface plasticity remain largely unclear. Understanding the hydrogen effect on interface plasticity and dislocation–grain boundary interactions is crucial for deciphering the mechanisms of hydrogen-induced degradation in lath martensite. This understanding is of both fundamental scientific and practical importance. In this study, we implement atomistic-scale modeling to investigate the effect of hydrogen on the sliding behavior of lath/block boundaries and the mechanisms that enable this sliding to occur. Additionally, we examine slip transmission and other local interactions between the dominant mobile $\frac{1}{2}[111]$ screw dislocation and lath/block boundaries in both pure and hydrogen-charged Fe and Fe–C alloys.

Remapping Through Direct Interpolation and Optimization for Finite Element ALE Hydrodynamics

B. Keith, D. Kim, B. Lazarov, C. Petra, M. Schmidt, V. Tomov

We propose a novel remapping approach tailored for Arbitrary Lagrangian-Eulerian (ALE) hydrodynamics. This method is well-suited for integration with ALE frameworks

capable of performing significant purely Lagrangian displacements between consecutive remesh/remap steps.
Given the initial and optimized meshes, we begin by performing a direct interpolation in physical space, bypassing the concept of PDE-based pseudotime advection. This approach is computationally feasible due to recent advancements in parallel, GPU-capable interpolation routines provided by the GSLIB library. The resulting interpolation ensures bounded fields with minimal diffusion but violates conservation. To restore conservation while preserving physical bounds, we employ two alternative optimization techniques. The first leverages interior point methods implemented via C. Petra's HiOp optimization library. The second technique builds on B. Keith's research on Proximal Galerkin Methods, performing optimization in a latent space that inherently avoids the need for explicit bounds constraints.
The proposed method produces minimal diffusion for finite element fields of arbitrary order and enables the direct remapping of quantities defined at integration points, eliminating the need to project onto finite element spaces. It circumvents challenges typically associated with synchronization between primal variables and conserved quantities in advection-based remap methods. We show results on standard 2D and 3D remap benchmarks and full ALE hydrodynamics simulations.
This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344 (LLNL-ABS-2002031).

Pointwise-in-time Error Bounds for a Fractional-derivative Parabolic Problem on Quasi-graded Meshes

S. Kelly, N. Kopteva

An initial-boundary value, subdiffusion problem involving a Caputo time derivative of fractional order $\alpha \in (0,1)$ is considered. The solutions of which typically exhibit a singular behaviour at initial time. We propose an extension to the approach, by Kopteva and Meng (SIAM J. Numer. Anal., 58, 2020), used to analyse the error of L1-type discretizations on both graded and uniform temporal meshes. We broaden the assumption on the regularity of the solution to incorporate more general solution behaviour, such that $|\delta_t^l u(\cdot,t)| \lesssim 1 + t^{\sigma-l}$ for some $\sigma \in (0,1) \cup (1,2)$ and any $l = 0,1,2$. Under this more general assumption on the solution, we give sharp pointwise-in-time error bounds on quasi-graded temporal meshes with arbitrary degree of grading (including uniform meshes, also considered Li, Qin, and Zhang (J. Comput. Math., 42 (2024)). Extensions to the semilinar case will also be considered.

Spectral Approaches to Fractional Derivatives

C. Klein, N. Stoilov

Fractional derivatives on the whole real line are often numerically approximated with Fourier techniques on the torus. We present an approach via Riesz fractional integrals on the whole real line with a multi-domain spectral method. The compactified real line is divided into a number of intervals. The integrals are computed with a Clenshaw-Curtis method after some transformations ensuring analytic integrands. As an example, solitary waves for fractional Korteweg-de Vries equations are computed. A comparison with results obtained with a discrete Fourier transform is presented. As an application, fractional nonlinear Schrödinger equations are discussed.

Low-order Preconditioning for High-order Finite Elements

T. Kolev, W. Pazner, C. Dohrmann, V. Dobrev, J.-S. Camier

High-order finite element methods provide a framework for accurately solving a spectrum of partial differential equations on general unstructured grids. These methods are particularly well-suited for modern supercomputers with GPU accelerators, where their efficiency and scalability rely on the adoption of partially assembled (PA) algorithms that reduce data motion during the application of high-order finite element operators.
However, the matrix-free nature of PA algorithms renders traditional preconditioning techniques, such as algebraic multigrid (AMG), inapplicable. This necessitates the development of new preconditioners tailored to the unique structure of PA operators. We introduce a robust class of such preconditioners: the low-order refined (LOR) methods for problems posed in H^1, $H(curl$, and $H(div)$ spaces. These preconditioners are constructed by deriving a spectrally equivalent low-order discretization of the high-order problem, thereby enabling the application of standard preconditioning techniques, such as AMG.
In this talk, we will describe the PA/LOR algorithms and their efficient implementation in the MFEM finite element library. Practical performance will be illustrated across a range of challenging applications.

Numerical Identification of Time-dependent Source in a Quasilinear Parabolic Equation

M.N. Koleva, L.G. Vulkov

We consider the problem of identifying the unknown source function $f(t)$ in the initial

boundary-value problem

$$
\begin{aligned}
&\frac{\partial u}{\partial t}-\frac{\partial}{\partial x}\left[a\left(\left(\frac{\partial u}{\partial x}\right)^2\right)\frac{\partial u}{\partial x}\right]=\varphi(x)f(t),\ (x,t)\in Q_T=\Omega\times(0,T),\ \Omega=(0,1),\\
&u(x,0)=u_0(x),\quad x\in\Omega, \qquad (1)\\
&\frac{\partial u}{\partial x}(0,t)=\frac{\partial u}{\partial x}(1,t)=0,\quad t\in(0,T],
\end{aligned}
$$

from the point observation

$$
\frac{\partial u}{\partial x}(x^*,t)=E(t),\quad t\in[0,T],\quad x^*\in\Omega. \qquad (2)
$$

Let $v=\frac{\partial u}{\partial x}$, $A(v)=a(v^2)v$. At the first stage, we reduce the inverse problem (1), (2) to the following loaded equation direct problem

$$
\frac{\partial v}{\partial t}-\frac{\partial^2 A\left(v\right)}{\partial x^2}+\frac{\varphi'(x)}{\varphi'(x^*)}\frac{\partial^2}{\partial x^2}(A(v(x,t))|_{x=x^*}=\frac{\varphi'(x)}{\varphi'(x^*)}E'(t), \qquad (3)
$$

$$
f(t)=\left(E'(t)-\frac{\partial^2}{\partial x^2}A(v(x,t))|_{x=x^*}\right)\left(\varphi'(x^*)\right)^{-1}, \qquad (4)
$$

$$
v(x,0)=u_0'(x),v(0,t)=v(1,t)=0. \qquad (5)
$$

Further, we drive a fourth-order in space difference scheme for the problem (3)-(5). The corresponding discrete inverse problem is solved by iterative algorithm. Finally, computational test examples are presented and discussed.

Dual-Weighted Residual Goal-Oriented Error Estimation For Space-Time Adaptivity In Phase-Field Fracture

V. Kosin, A. Fau, F. Hild, T. Wick

This presentation focuses on space-time adaptivity for phase-field fracture problems. The methodology requires a space-time formulation and utilizes a space-time Galerkin finite element discretization for the governing phase-field equations. Then, goal functionals (i.e., quantities of interest) are introduced. The computational implementation of goal-oriented error control employs the dual-weighted residual method in which an adjoint problem must be solved. As the temporal derivative only appears in the irreversibility constrained, lagrange multiplicators are introduced in combination with an active set method. Then, the primal and the adjoint problem contain a temporal derivative, such that general goal functionals can be considered. The temporal and spatial errors are localized using a partition of unity, which allows one to adaptively refine and coarsen the time intervals and space elements in the space-time cylinder. Numerical tests are performed on a single edge notched tensile and shear test to investigate the quality of the proposed error estimator.

Non-overlapping DD-BURA Preconditioning on Unstructured Tetrahedral Meshes

N. Kosturski, S. Margenov, Y. Vutov

Finite element method (FEM) on unstructured meshes has proven to be an indispensable tool in computer modelling. Large-scale simulations and complex models require parallel computing. We analyse the performance of a non-overlapping domain decomposition (DD) preconditioner for finite element method (FEM) discretisation of the Poisson equation $-\Delta u = f$ in the polyhedral domain $\Omega \subset \mathbb{R}^3$. ParMETIS is used to partition the mesh into subdomains $\Omega_i, i = 1, 2, \ldots, p$ with interface γ.
For the preconditioning of the obtained linear system, a block factorization of the matrix A is used. The blocks correspond to the degrees of freedom internal to Ω_i and those on γ. The inverse of the Schur complement, corresponding to the unknowns on γ is approximated using the best uniform rational approximation (BURA) of order k of $\Lambda^{-1/2}$, where Λ is the discretisation of the Laplace-Beltrami operator on the interface γ. The inverses of the blocks, corresponding to the unknowns internal to Ω_i can be computed without any communication.
Experimental results confirming the theoretical asymptotic optimality of the proposed preconditioner are presented. Several nested meshes with the same and with different partitionings are used. Further, the effects of the accuracy of the inner solvers used, as well as the order of the BURA approximation on the performance of the preconditioner, are studied.

On The Small-Time Local Controllability Of A Class Of Polynomial Systems

M.I. Krastanov, M.N. Nikolova

Small-time local controllability (STLC) is one of the basic properties of a nonlinear control system. It is crucial for solving different problems of the mathematical control theory. We follow a general geometrical approach proposed by Hermann, Hermes, Kawski, Krener, Sussmann, and etc. It is based on using different differential-geometric tools as the classical formula of Campbell-Baker-Hausdorff formula (taken from the Lie group theory), different symmetries (related to the structure of the control values), and etc.

Consider the following control system Σ on R^n

$$\dot{x}(t) = f(x(t)) + u(t),$$

$$x(0) = 0,\ u(t) \in U \cap \bar{\mathbf{B}}$$

where U is a closed convex cone in R^n, $\bar{\mathbf{B}}$ is the closed unit ball of R^n centered at the origin and $f : R^n \to R^n$ is a map whose components are polynomials which are homogeneous of second degree. The reachable set $\mathbf{R}(x_0, T)$ of Σ is the set of all points reachable in time not greater than T by means of admissible trajectories of Σ starting from the point x_0. The control system is called small-time locally controllable at the point x_0 iff x_0 belongs to the interior of the reachable set for each $T > 0$.

Our approach is based on a suitable definition of a set $E^+(x_0)$ of tangent vector fields to the reachable set of a control system at the starting point x_0. The basic idea is that if the origin belongs to the interior of the convex hull of $E^+(x_0)$ then the corresponding control system is STLC at the point x_0. We study carefully the Lie algebra of the vector fields generated by the drift term f of the control system Σ and the constant vector fields generated by the set $U \cap \bar{\mathbf{B}}$. We prove that some "bad Lie brackets" (in the sense of Sussman) belong to the set $E^+(0)$, and hence they are not obstructions for small-time local controllability. As a corollary we obtain a new sufficient condition for the small-time local controllability of the control system Σ at the origin.

Non Degeneracy of Optimality Conditions

M. Krastanov, N. Ribarska

A Mayer optimal control problem is studied under pure state constraints. A necessary and sufficient condition for non degeneracy of Pontryagin maximum principle is obtained.

Constrained Infinite-Time Horizon Linear Quadratic Optimal Control under Uncertainty

M.I. Krastanov, R. Rozenov, B.K. Stefanov

We consider a linear-quadratic differential game played over an infinite-time horizon, where the minimizing player's controls are subject to specific constraints. To address the challenges arising from the constraints, we propose an approach that transforms the original infinite-horizon game into a suitable finite-time horizon problem. The results offer new insights into the structure of robust control strategies in dynamic games with constrained control variables, contributing to the design of more effective and practical solutions in such settings.

Parameter-robust Preconditioner for a Classical Formulation of the Stokes-Darcy Problem

J. Kraus

We consider a classical formulation of the Stokes-Darcy interface problem with Neumann-Neumann coupling and construct a fully parameter-robust norm-equivalent preconditioner within an abstract framework for the stability analysis of perturbed saddle-point problems. The construction involves a simple norm-fitting technique and results in a two-by-two block-diagonal preconditioner for the system with the Stokes velocity and the vector of Stokes and Darcy pressures as unknowns. We discuss the implementation of this preconditioner and, furthermore, show some numerical tests.

2-Rotund Norms for Generalized Baernstein Spaces and Their Duals

D. Kutzarova

We consider a generalized Baernstein space associated to a compact family of finite subsets of an uncountable set. We show that for certain transfinitely defined families such spaces admit an equivalent 2-rotund norm. We also show that for an arbitrary family the dual space admits an equivalent 2-rotund norm. The results are joint with S.J. Dilworth.

State-based Numerical Solution of PDE-constrained Optimal Control Problems

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

We consider an abstract framework for the numerical solution of optimal control problems (OCPs) subject to partial differential equations (PDEs). Examples include not only the distributed control of elliptic PDEs like the Poisson equation but also initial-boundary value problems (IBVPs) for parabolic and hyperbolic equations as well as boundary control problems. The approach covers the standard L_2 regularization as well as the more general energy regularization. We reduce the OCPs to variational problems in the state from which the optimal control can easily be recovered. Moreover, we will also include state and control constraints leading to variational inequalities for the state.
We use the Galerkin method as the overall discretization technique that is nothing but the usual finite element method (FEM) in the case of elliptic boundary value problems, and the fully unstructured space-time FEM for parabolic and hyperbolic IBVPs. We discuss regularization and finite element (fe) error estimates, and derive an optimal relation between the regularization parameter and fe mesh-size in order to balance the accuracy

and the energy costs for the corresponding control. Adaptive versions can easily be derived on the basis of the computable L_2 error between the computed fe state and the known desired state. Here the regularization may be adapted to the local mesh-size that can vary considerably in these adaptive finite element methods (AFEM).

Finally, we also discuss efficient (parallel) solvers for the resulting algebraic systems of fe equations, and their use in a nested iteration procedure that is controlled by the accuracy of the fe approximation to the desired state and the energy cost of the recovered control.

We present numerical results for benchmark OCPs with different features illustrating the theoretical findings quantitatively.

Polynomial Algorithm for Minimum Complete Pareto Front of a Biobjective Minimum Spanning Trees Problem

L.M. Laskov, M.M. Marinov

The goal of this research is to provide a description of the set of all Pareto optimal solutions of the biobjective minimum length minimum risk spanning trees problem. In the extreme case in which the given network is such that for all edges respectively the length weights are equal and the risk weights are equal, then each spanning tree of the network is also a Pareto optimal spanning tree. Therefore, the number of Pareto optimal spanning trees can be n^{n-2}, where n is the number of vertices of the network. This shows that for large networks, methods that construct representation of the set of all Pareto optimal trees, are of great interest. Such an representation can be given by the *minimum complete Pareto front*, which is the set composed from single representative of each of the K number of classes of equivalent Pareto optimal solutions. We will note that as the size of the network increases, so does the number of elements of the minimum complete Pareto front.

In this paper we propose an *exact method* that constructs the minimum complete Pareto front of the biobjective minimum spanning trees problem in which the first objective function is a linear and represents minimum length, and the second objective function is a nonlinear bottleneck function and represents minimum risk. The proposed algorithm has a *polynomial computational complexity* that allows it application in case of large networks.

For large networks the number of classes of equivalent Pareto optimal solutions K may grow significantly, and in this case the algorithm allows to construct a predefined number n_0 of elements of the minimum complete Pareto front. We prove that the computational complexity of the algorithm is $O(s(m+n\lg n))$, where the parameter $s=\min\{n_0, K\}$. As n_0 increases, the feasible objective region decreases until the last element of the minimum complete Pareto front is constructed.

We prove the correctness of the proposed algorithm analytically and we verify it with the results of our experiments. Also, we verify our implementation with various large random networks.

Large Scale Parallel Topology Optimization of Time Harmonic Dynamic Problems

B. Lazarov, M. Schmidt

Today, topology optimization is a key tool in the mechanical, automotive, and aerospace industries.The fundamental idea is to distribute material within a predefined domain by minimizing a chosen objective and meeting a set of constraints, such as minimizing power dissipation or maximizing heat transfer subject to a limited amount of material. The optimization problems are discretized, and the solution process involves repeated system analyzes, gradient evaluation steps using adjoint sensitivity analysis, and design updates based on mathematical programming methods. The result of the topology optimization procedure is a bitmap image of the design leading to design freedom unmatched by any other approach. However, this freedom comes at the cost of substantially increasing the required computational power. Finer discretizations provide better design descriptions while demanding the use of large parallel machines. The size of the discrete problems necessitates the deployment of iterative techniques with convergence hindered by the sharp contrast between the properties of the different constituent materials and the ill-conditioned number of the discretized system of equations due to the problem size. Therefore, most of the results reported in the literature utilize direct solvers, limiting the studies and the rest to academic 2D examples.
Our work extends and demonstrates topology optimization to large-scale 3D linear elastic problems exited by time-harmonic loads. Their discretizations result in large, complex linear systems of equations that are notoriously difficult to precondition and solve. To this end, we reformulate the discrete linear systems in equivalent real-valued two-by-two block systems, which are relatively easy to precondition and solve. Several different solution strategies are demonstrated on 2D and 3D topology optimization problems implemented with the help of the MFEM finite element discretization library, focusing on scalability and the impact of material contrast.
This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

On Operator Preconditioning for Condensed Hybridized Systems

J. Lee

Static condensation with hybridization is a popular finite element method technique to reduce the number of global unknowns of linear systems. The condensed system is mathematically equivalent to the original linear system but construction of preconditioners for condensed linear systems needs a separate study. In this talk we present an operator preconditioning approach for condensed linear systems leading to construction of parameter-robust preconditioners. We show two examples of the framework, one for hybridized dual mixed reaction-diffusion equations and the other for hybridized discontinuous Galerkin methods for the incompressible stationary Stokes equations.

The talk is based on a joint work with Sander Rhebergen and Esteban Henriquez (University of Waterloo).

An Augmented Lagrangian Preconditioner for the Control of the Navier–Stokes Equations

S. Leveque, M. Benzi, P. Farrell

Optimal control problems with PDEs as constraints arise very often in scientific and industrial applications. Due to the difficulties arising in their numerical solution, researchers have put a great effort into devising robust solvers for this class of problems. An example of a highly challenging problem attracting significant attention is the distributed control of incompressible viscous fluid flow problems. In this case, the physics is described by the incompressible Navier–Stokes equations. Since the PDEs given in the constraints are non-linear, in order to obtain a solution of Navier–Stokes control problems one has to iteratively solve linearizations of the problems until a prescribed tolerance on the non-linear residual is achieved.
In this talk, we present efficient and robust preconditioned iterative methods for the solution of the stationary incompressible Navier–Stokes control problem, when employing a Gauss–Newton linearization of the first-order optimality conditions. The iterative solver is based on an augmented Lagrangian preconditioner. By employing saddle-point theory, we derive suitable approximations of the (1, 1)-block and the Schur complement. Numerical experiments show the effectiveness and robustness of our approach, for a range of problem parameters.

A New Rational Approximation Algorithm via the Empirical Interpolation Method

Y. Li

In this talk, I will present a rational approximation algorithm via the empirical interpolation method for interpolating a family of parametrized functions, leading to numerical algorithms for space-fractional differential equations, parameter-robust preconditioning, and evaluation of matrix functions. In addition, I will provide a convergence estimate of this algorithm using the metric entropy numbers.

Numerical Simulation of Propagation of Uncertainties in Coastal Aquifers

D. Logashenko, A. Litvinenko, R. Tempone, G. Wittum

Simulation of salinization of coastal aquifers plays an important role in prediction of availability of water resources. Uncertainty in hydrogeological parameters may affect the groundwater flow and significantly reduce accuracy of the prediction of the pollution transport. In this talk, we present numerical approaches for estimation of propagation of the uncertainty from the parameters to the solution in the subsurface density-driven flow models represented by a system of non-linear PDEs. We consider model problems with random fields of porosity and permeability that represent the limited knowledge of the data. We construct a low-cost generalized polynomial chaos (gPC) expansion surrogate model. Computation of the gPC coefficients is performed by projection on sparse tensor grids. Furthermore, we consider a multilevel Monte-Carlo technique (MLMC) and investigate its efficiency for this type of the non-linear problems. Parallelization is applied to both the numerical solution of the deterministic problems (scenarios) and the high-dimensional quadrature over the parametric space. We present results of the parallel computations of 2d and 3d aquifers.

Kinetic Multiphase Model And Full Coupled Implicit Scheme For Large-scale Subsurface Carbon Sequestration Simulation

S. Lu, D. Logashenko, S. Matthai, A. Nägel, G. Wittum

To fully understand and correctly predict the behavior of CO2 storage, accurate mathematical models and advanced large-scale reservoir simulation numerical schemes need to be developed. We propose a kinetic multiphase model that accounts for the kinetics of mass transfer between the carbonic and aqueous phases. This inclusion introduces dynamic changes in the density of fluid phases, driving density-induced flows. Unlike standard equilibrium models, this model eliminates the first-order dependence of dissolved CO_2 on mesh refinement. Solving multiphase models is challenging, especially for large-scale over long periods. However, most discretization schemes are explicit or semi-implicit which restricts the time step size of the simulations. In this work, a fully coupled and implicit framework is proposed for large-scale simulations of miscible multiphase flow in heterogeneous porous media. Vertex Centered Finite Volume Method is employed for the spatial discretization of the mass conservation equations. To address the time discretization issue we employ, for the first time, the linearly implicit extrapolation scheme (LIMEX) to solve the highly non-linear coupled two-phase model. To solve the arising large sparse systems of linear equations, we apply the geometric multigrid (GMG) method that demonstrates optimal, linear complexity and allows an efficient parallelization on supercomputers. The parallel scalability of our simulation framework is demonstrated using an implementation based on the UG4 platform. Proof-of-concept results successfully capture critical features of CO_2 migration, including filtration through capillary barriers and convective dissolution of CO_2 at the base of the plume.

Spectrally Enriched Additive Average Schwarz For The Parabolic Multiscale Problem

L.F. Lund, L. Marcinkowski, T. Rahman

In this paper, we demonstrate the additive average Schwarz method applied to the multiscale time-dependent heat equation by using a spectrally enriched coarse space. We state that the condition number depends on the mesh parameter ratio $\frac{H}{h}$, and is independent of the time step size τ, if all necessary eigenvectors are used in the spectral enrichment. We confirm these results on a multiscale coefficient distribution with different mesh and time parameters.

An Adaptive Average Schwarz Method for a Morley Multiscale 4th Order Problem

L. Marcinkowski, T. Rahman

In this paper, we describe and analyze an Average Schwarz Method with spectrally enriched coarse space for a non-conforming Morley finite element discretization of a 4th-order elliptic multi- scale problem. The derived symmetric preconditioner is applied and the PCG iterative method is used to solve the preconditioned problem. If the enrichments of the coarse space contain sufficiently many specially constructed eigenfunctions, then the convergence rate of the PCG method is weakly dependent on the ratio of the coarse to fine mesh h/H. The results are extensions of the works of the 2nd author in which there was presented and analyzed the average Schwarz method for a classical non-multiscaled fourth order problem.

Mathematical Challenges of Modeling the Fluid Flow of the Brain - Brain Clearance, Sleep and Dementia

K.-A. Mardal

Recent theories suggest that a fundamental reason for sleep is simply clearance of metabolic waste produced during the activities of the day. A crucial component of these theories are the fluid flow within and around the brain, in health and disease.

In this talk we will present multi-physics problems and numerical schemes that target these applications. In particular, we will be lead from basic applications of neuroscience into multi-physics problems and interfaces coupled problems involving Stokes, Biot, and Darcy problems for describing the fluid-structure interaction between the brain and its fluids. Particular focus for us has been the exploitaton of fractional solvers at the brain-fluid interface for creating efficient monolitic solvers.

BURA-AMLI Numerical Solution of Fractional Diffusion Problems

S. Margenov

The talk is devoted to the numerical solution of the linear system $\mathbb{A}^\alpha \mathbf{u} = \mathbf{f}$, $\alpha \in (0,1)$, where $\mathbb{A} \in \mathbb{R}^{N\times N}$ is a properly scaled matrix obtained from a finite element approximation of second-order elliptic problems in $\mathbb{R}^2$. Under these assumptions, $\mathbb{A} = \mathbb{M}^{-1}\mathbb{K}$, where $\mathbb{K}$ and $\mathbb{M}$ are the stiffness and mass matrices. Then $\mathbb{A}$ is symmetric and positive definite with respct to the energy inner product associated with $\mathbb{M}$. The matrix $\mathbb{A}^\alpha$ is also symmetric, positive definite, and dense, which is consistent with the nature of spectral fractional diffusion. We apply the BURA method to solve the nonlocal fractional linear system, see [1]. The numerical solution is based on the best uniform rational approximation $r_{\alpha,k}(z)$ of power k of z^α for $z \in [0,1]$. Then $\mathbb{A}^{-\alpha} \approx \lambda_1^{-\alpha} r_{\alpha,k}(\lambda_1 \mathbb{A}^{-1})$ where $\lambda_1 > 0$ is the first eigenvalue (or its approximation) of $\mathbb{A}$. The BURA method reduces the solution of the dense-matrix linear system to the solution of k systems with sparse matrices of the form $\mathbb{K} - \tilde{d}_i\mathbb{M}$, $\tilde{d}_i < 0$, $i = 1,\dots,k$. The solver for these auxiliary diffusion reaction systems plays a key role in the computational efficiency of the method.

We integrate the AMLI (Algebraic Multilevel Iteration) method (see [2] and references therein) into the BURA structure. We call the resulting composite method BURA-AMLI. The construction of AMLI is based on two-level recursive hierarchical block representations. The constant in the strengthened CBS (Cauchy-Buniakowski-Schwartz) inequality controls the condition number of the corresponding two-level and multilevel preconditioners. A key issue here is the robustness of the estimates with respect to the reaction parameter $-\tilde{d}_i$. Optimality conditions for the AMLI preconditioners are obtained for the considered uniform and local mesh refinements. We thus show $O(\log^2 NN)$ estimates of the computational complexity of the composite BURA-AMLI algorithms.

References

[1] Harizanov, S., Lazarov, R., Margenov, S.: A survey on numerical methods for spectral Space-Fractional diffusion problems. Fractional Calculus and Applied Analysis. **23** (6) (2021). 1605-1646

[2] Kraus, J., Margenov, S.: Robust Algebraic Multilevel Methods and Algorithms. Radon Series on Computational and Applied Mathematics. **5**, de Gruyter (2009), p. 246

The Walk on Spheres Monte Carlo Algorithm for Solving Partial Differential Equations

M. Mascagni

The stochastic representation to the solutions of partial differential equations (PDEs) and integral equations (IEs) has been known for decades. These representations have lead to a variety of Monte Carlo methods for the numerical solution of both PDEs and IEs, among them is a method called the Walk on Spheres (WoS) algorithm. WoS has been quite successful in solving linear elliptic and parabolic PDEs with Dirichlet boundary conditions in a very cost effective way. This numerical analysis work was taken up by the computer graphics community, who are experts in Monte Carlo through their use of it in image rendering via ray tracing. Their interest stems from the fact that WoS and ray tracing both permit the representation of the geometry of the problem in a very compact and computational efficient way via Bounding Volume Hierarchy. This has lead to the expansion of the scope and efficiency of WoS in a wide variety of ways which will be presented here.

On the Implementation of Algorithms for the Subset Sum Problem

A. Mucherino, J-H. Lin

Given a set S of integer numbers and a target integer value t, the Subset Sum Problem (SSP) asks whether there exists a subset of S for which the sum of all its elements corresponds to the given target t. The SSP is one of Karp's 21 famous **NP**-complete problems, and it is widely studied in the scientific literature because of its large range of applications.

The SSP search space can be seen as a binary tree where the inclusion (or exclusion) of each of the integers in S (associated to the current tree layer) in potential subsets is selected at each branching point, so that a complete path (from root to leaf node) on the tree actually represents one SSP solution. An exhaustive search on this binary tree leads therefore to the definition of a simple, yet effective, algorithm for the SSP, which has however an exponential worst-case complexity.

Even if there should be no algorithmic solutions capable to exhibit a polynomial complexity w.r.t $n = |S|$ (unless $\mathbf{P} = \mathbf{NP}$, which is unlikely), there are algorithms exhibiting lower-than-exponential complexity for certain sub-classes of SSP instances. For example, algorithms were proposed for the SSP that are based on a dynamic programming approach, where it is claimed that the complexity is polynomial w.r.t the value of the target t. We talk in this case of *pseudo* polynomial complexity.

The present work stems from the observation that a significant gap exists between the theoretical advancements and the practical implementations of these algorithms. Moreover, in many of the algorithms we were able to review up to now, the theory behind the complexity of a given algorithm does not seem to take into explicit consideration the actual computational complexity of the operations that the algorithm is supposed to perform. As a consequence, we have found examples of SSP algorithms where the theoretical complexity does not really match with the computational time of the corresponding implementations. In parallel, we are exploring modern programming paradigms, as well as the use of quantum technologies, for a more effective implementation of these algorithms for the SSP.

On the Error Bounds of the Gauss-Type Quadrature Formulae Associated with Spaces of Parabolic and Cubic Spline Functions with Double Equidistant Knots

G. Nikolov, P.B. Nikolov

In two papers from 1995 P. Köhler and G. Nikolov showed that Gauss–type quadrature formulae associated with spaces of spline functions with equidistant knots are asymptotically optimal in certain Sobolev classes of functions. In particular, Gauss–type quadratures associated with the spaces of spline functions of degree $r-1$ with double equispaced knots are asymptotically optimal definite quadrature formulae of order r when r is even, and it is conjectured that the asymptotical optimality property persists also in the case of odd r. For $r = 3$, 4, these quadrature formulae have been constructed by G. Nikolov, who also proved estimates for their error constants. We refine the estimates for the error constant in the case $r = 3$, and to point out to some error estimates in both cases $r = 3$ and $r = 4$, which are easier to evaluate and could be sharper than those which involve the uniform norm of the r-th derivative of the integrand.
Based on a joint work with Geno Nikolov.

A Posteriori Algebraic Error Estimates and Nonoverlapping Domain Decomposition in Mixed Formulations: Energy Coarse Grid Balancing, Local Mass Conservation on Each Step, and Line Search

M. Bastidas Olivares, A. Beni Hamad, M. Vohralík, I. Yotov

We consider iterative algebraic solvers for the saddle-point mixed finite element discretizations of the model Darcy flow problem. We propose a posteriori error estimators of the algebraic error as well as a nonoverlapping domain decomposition algorithm. The estimators control the algebraic error from above and from below in a guaranteed and fully computable way. The distinctive feature of the domain decomposition algorithm is that it produces a locally mass conservative approximation on each iteration. Both the estimate and the algorithm rely on a coarse grid solver, a subdomain Neumann solver, and a subdomain Dirichlet solver. The algorithm also employs a line search to determine the optimal step size, leading to a Pythagoras formula for the algebraic error decrease in each iteration. Numerical experiments illustrate the theoretical developments and confirm the efficiency of the algebraic error estimates and of the domain decomposition algorithm.

Sensitivity Analysis of the Unified Danish Eulerian Model with a Focus on Robust Variance-Based Techniques

T. Ostromsky, V. Todorov, I. Dimov

Environmental models, such as the Unified Danish Eulerian Model (UNI-DEM), play a pivotal role in assessing air pollution dynamics and guiding policy decisions aimed at mitigating adverse environmental and health effects. Understanding the influence of input parameters on model outputs is crucial for improving model reliability, identifying key variables with major impact on certain output results. Moreover, it is helpful too in optimizing the use of computational resources, which are quite significant in many long-term simulations. Variance-based sensitivity analysis has emerged as a robust framework for quantifying the contribution of input uncertainties to the variability of model outputs. This study focuses on applying a robust Monte Carlo stochastic approach to perform variance-based sensitivity analysis of UNI-DEM.

The Unified Danish Eulerian Model is a comprehensive tool for simulating the spread, long-range transport, chemical transformations, and deposition of a large number of atmospheric pollutants. Due to the complexity of its chemical mechanism, meteorological data inputs, and spatially resolved domain, UNI-DEM involves numerous parameters with significant variability. These parameters include emissions data, chemical reaction rates, meteorological conditions data, etc. The challenge lies in identifying the most influential parameters while accounting for their uncertainties to ensure accurate and computationally efficient predictions.

In this paper, we employ a Monte Carlo-based sensitivity analysis approach to evaluate the impact of input parameters on UNI-DEM outputs. To reduce the computational efforts associated with high-dimensional input spaces, quasi-random methods such as Sobol sequences are utilized. These methods ensure better convergence compared to traditional random sampling. A thorough robustness check of the Monte Carlo approach is conducted to ensure that the sensitivity estimates are reliable. vely small sensitivity indices in terms of accuracy and efficiency.

About Parallelization of Algorithm for Computation of Covering Radius of Linear Codes

M. Pashinska-Gadzheva, I. Bouyukliev

The covering radius is one of the important characteristics of linear codes. It provides information about whether the code is suitable for use in data compression and noise reduction algorithms. It is also used in algorithms for generating and classifying linear codes. Thus, its computation is included in many computer algebra systems such as MAGMA. The problem is known to be NP-complete. There are different methods for computation of the covering radius. One approach uses the dual code for the computations. It works for codes with small codimension. Furthermore, it has great space complexity in terms of implementation.

In the current work we consider algorithm that uses the cosets of the linear code with given generator matrix in standard form and its parallelization. The algorithm computes the distance between the linear code and each of its cosets. For this purpose, all vectors of the nonproportional costes must be generated. Thus, it can also be used for the computation of the coset distance distribution.

We present three directions for the parallelization of the algorithm. Firstly, computations are executed for a multiple cosets at the same time. Secondly, we parallelize the algorithm for the generation of the vectors included in each coset. The parallelization is implemented for shared and distributed memory systems using MPI and/or OpenMP. For the implementation in shared memory system using OpenMP, we parallelize a recursive algorithm using use the *task* construct. Lastly, further optimization can be used for the computation of each vector using vectorization. Such parallelization with extended vector registers can be added to implementations on both shared and distributed memory systems. The parallelized implementations have been executed on two hardware platforms. Using a set of linear codes with different parameters we evaluate the performance of these parallelization directions.

On a Decoupled Solver for Biot's Model

Á. Pé de la Riva, F.J. Gaspar, X. Hu, J. Adler, C. Rodrigo, L. Zikatanov

In this work, we propose an iterative solver for the quasi-static Biot's model for soil consolidation. Our approach first solves the flow problem, followed by the mechanics, in a manner similar to the so-called fixed-stress splitting method. The appearance of non-physical oscillations in the pressure approximation of Biot's model for poroelasticity under low permeabilities and/or small time steps is a well-known issue. Thus, we introduce a novel stabilization that eliminates spurious oscillations and also ensures the con- vergence of the iterative solver. Finally, we will show some numerical results to demonstrate the efficiency and robustness of our solver with respect to both discretization and physical parameters.

Software Energy Efficiency Towards Sustainable Computing

K. Penev

The increasing dependence on information technology in many aspects of human life often causes high demand for resources, in particular energy, which has an impact on the environment obeying natural, physical limitations. Global sustainability requires efficient responsible computing and improvement of hardware and software energy efficiency. This article focuses of software energy efficiency and its role towards sustainable computing. The introduction points out Bremermann's limit and the possible consequences if extensive improvements in computing performance approach this limit. The role of green energy-efficient software applied to large-scale tasks is analyzed. An empirical investigation illustrates the energy efficiency of different algorithms in solving identical conventional tests. The summarized large-scale experimental results of these tests and a consideration of further work conclude the article.

Ethical Problems in Modeling Disaster Situations

V. Ivanov, E. Penkov, N. Bozakova, S. Fidanova

This article examines the ethical issues surrounding disaster preparedness and response. Several key ethical issues in the context of disasters are addressed, including the equitable distribution of limited resources such as vaccines, medical supplies, and personnel. Emphasis is placed on awareness and protection of vulnerable groups, as well as the balance between urgent needs and ethical standards. It also examines the ethical implications of humanitarian dependency in disaster settings, proposing a shift in focus from dependency to empowerment based on the resilience of affected communities. When modeling a disaster situation and its consequences, it is particularly important to take ethical principles into account in order to minimize damage and achieve better results. Such a model could be used by governments, health authorities, social services and humanitarian organizations to prepare for and respond to global health crises.

Enabling Digital Twins in Process Engineering Through Reduced-order Surrogate Modeling

L. Peterson, A. Forootani, E.I. Sanchez Medina, I.V. Gosea, P. Benner, K. Sundmacher

Being deemed as an emerging technology in modern times characterized by fast and reliable computational frameworks, digital twins (DTs) are gaining unprecedented attention because of their advantages in numerous fields of applied sciences. Here, we mention

only a few of their features, e.g., to optimize process design, quality control, health monitoring, reliable decision-making, etc. This is performed by comprehensively modeling the physical world as a group of interconnected digital models, that compose the digital counterpart, or in short, the DT. In the context of process and chemical engineering, the advantages of DTs are on the verge of achieving ubiquitous recognition. For example, in the context of CO_2 catalytic methanation reactors (the "physical twins"), DTs can indeed provide advanced, reliable solutions for monitoring and controlling such reactors under variable conditions. This enables safer, optimized reactor performance in real-time operation mode. The approach pursued in our work relies on computing fast, accurate models to predict optimal coolant temperature and prevent overheating.
We investigate and compare several reduced-order surrogate modeling techniques: a graph attention network (GAT) architecture, a reduced-order modeling and learning approach known as operator inference (OpInf) with stability guarantees, and a sparse regression technique with greedy sampling (SINDy). These methods are evaluated for their ability to model the dynamic operation and control of our test case. We compare the accuracy and computational efficiency of these surrogates to identify models that can improve renewable energy conversion processes. The goal is to identify promising candidates for constructing a DT of the reactor, which will be used to optimize its operation and facilitate its integration into functional renewable energy systems.

A Time–Adaptive Optimisation–Based Domain–Decomposition Algorithm for Fluid–Structure Interaction Problems

I. Prusak, D. Torlo, M. Nonino, G. Rozza

Fluid-Structure Interaction (FSI) problems, which describe the dynamic interplay between a fluid and a solid, present significant mathematical challenges due to the complex coupling at the fluid–structure interface. This interface, shared by the fluid and solid subdomains, evolves based on the dynamics of both, making its profile unknown a priori. Despite extensive research, a unified mathematical approach to FSI remains elusive, partly due to the intricate nature of the Navier-Stokes and elastic solid equations that govern the problem.
Traditionally, FSI problems are tackled using either partitioned or monolithic approaches. Partitioned algorithms leverage existing computational tools for fluid and structural dynamics, coupled through iterative procedures, while monolithic algorithms solve the coupled problem simultaneously by imposing global fluid-structure spaces. Although partitioned approaches are computationally advantageous and highly parallelisable, they often suffer from stability and convergence issues, particularly due to the "added-mass" effect common in cardiovascular applications.
Given the complexity of FSI problems and the need for very small time steps to achieve numerical convergence, employing time–adaptive strategies is essential in many scenarios where computational costs escalate rapidly. Building on the limitations of traditional methods, we propose a time − adaptive partitioned optimisation–based algorithm designed to ensure stable coupling of interface conditions between fluid and solid subdo-

mains. To this end, we employ a custom local time estimator for pressure-dominated flows, which are especially challenging due to the differential–algebraic structure of the fluid subproblem. Furthermore, incorporating time–adaptivity entails a search for more effective optimisation algorithms capable of overcoming the local and slow convergence of classical minimisation methods. In this context, trust-region methods are employed to improve robustness and convergence by adaptively managing the optimisation process.

Efficient Splitting Methods for Flow in Deformable Porous Media

F.A. Radu

We will present robust and efficient fixed-stress type splitting solvers for fully coupled flow and deformation in porous media. The considered mathematical model will be based on the quasi-static, linear Biot equations. Stabilization and optimization of the fixed-stress scheme will be briefly discussed. A new family of splitting schemes based on approximate Schur complement and a fixed-stress type scheme for a nonlinear Biot model will be then detailed presented.

Space-Time Finite Element Methods in Thermo-Elastodynamics

M. Reichelt, O. Steinbach

We present a novel approach for the thermo-elastic coupling using space-time finite elements. This method enables the simultaneous simulation of heat transfer and structural mechanics in a fully coupled manner. We will discuss the mathematical formulation of this approach, highlight its advantages, and present numerical examples that demonstrate its accuracy and computational efficiency in analyzing multiphysics systems. We will also cover recent developments, challenges, and future directions in this area.

A Semi-Analytic Diagonalization FEM for the Spectral Fractional Laplacian

A.J. Salgado, S.E. Sawyer

We present a technique for approximating solutions to the spectral fractional Laplacian, which is based on the Caffarelli-Silvestre extension and diagonalization. Our scheme uses the analytic solution to the associated eigenvalue problem in the extended dimension. We show its relation to a quadrature scheme. Numerical examples demonstrate the performance of the method.

Adaptive LOD BDDC for Elliptic Problems with Rough Coefficients

M. Sarkis

We consider finite element methods of multiscale type to approximate solutions for two-dimensional symmetric elliptic partial differential equations with very rough coefficients. The methods are of Galerkin type and follow the Variational Multiscale and Localized Orthogonal Decomposition–LOD approaches in the sense that it decouples spaces into multiscale and fine subspaces. In a first method, the multiscale basis functions are obtained by mapping coarse basis functions, based on corners used on primal iterative sub structuring methods, to functions of global minimal energy. This approach delivers quasi-optimal a priori error energy approximation with respect to the mesh size, but it is not robust with respect to high-contrast coefficients. In a second method, edge modes based on local generalized eigenvalue problems are added to the corner modes. As a result, optimal a priori error energy estimate is achieved which is mesh and contrast independent. The methods converge at an optimal rate even if the solution is only in H^1. Numerical experiments will be provided. This is a joint work with Alexandre Madureira, LNCC, Brazil.

Modeling Groundwater Flow and Nuclide Transport in Fractured Media with d^{3}f++

A. Schneider, H. Zhao, D. Logashenko, J. Wang, A. Nägel,
M. Knodel, G. Wittum

The international DECOVALEX program ("development of coupled models and their validation against experiments", since 1992) is focused on coupled thermal, hydrological, mechanical, and chemical processes relevant to deep geologic disposal of nuclear waste. The primary objective of the "PA TASK" in the current phase DECOVALEX 2027 is to build confidence in the models, methods and software used for post-closure performance assessment (PA). This is achieved through a staged comparison of the models and methods used by the participating teams. Several benchmarks and a generic reference case describing a repository for spent nuclear fuel (SNF) in a fractured crystalline host rock are systems for comparison. GRS started last year participating in the modeling of two benchmarks and the reference case applying the code d^{3}f++ (distributed density driven flow, Schneider et al. 2023), based on the ug4 simulation framework (Vogel et al. 2014). The four fractures benchmark is based on a cubic model domain with four explicitly defined fractures with distinguished apertures and parameters. The spaces between these fractures are filled with another dfn consisting of minor fractures, defined by stochastic parameters. The reference case is similarly structured with six determined fractures and, additionally, three layers with differing parameters and a repository with complex geometry. In both models, groundwater flow is driven by a pressure gradient, and sorbing and decaying tracers are released from varying sources. In our d^{3}f++ models, the main fractures are realized as lower-dimensional objects of discrete fracture networks (dfn). Minor fractures are generated using FracMan (Golder 2018) and, finally, are represented by an equivalent porous medium (epm). Results are presented for flow and transport simulations using LIMEX algorithms (Nägel et al. 2019) up to multigrid level 1 and 2 (5 million grid elements). The preliminary results match very well with the results of the other teams.

First-Order Form of Dynamic Poroelasticity: Tailored Discretization and Solver

P. Shamko, M. Anselmann, M. Bause

The numerical simulation of flow in deformable porous media modeled by a coupled system of hyperbolic and parabolic partial differential equations, referred to as the dynamic Biot system, is addressed. The mathematical model is rewritten as a **first-order in space and time evolutionary problem**. In this multi-field formulation, the stress tensor, the time derivative of the displacement variable, the pressure head and the fluid flux are the unknown variables. A **structure preserving numerical approximation** of the first-order form is developed. The mathematical characteristics of the system are inherited to its fully discrete counterpart. The approximation of the stress and flux variable is part of the discretization itself. An advantage of this formulation is the direct accessibility of these variables, which may hold physical relevance.
Well-posedness of the evolutionary problem is ensured by an abstract solution theory in exponentially weighted Bochner spaces. For the discretization, we propose **space-time finite element methods (STFEMs) of arbitrary order** based on **discontinuous Galerkin** techniques. To preserve the mathematical structure, penalization and correction terms are added. Well-posedness of the discrete system is guaranteed by the abstract solution theory again. **Optimal order error estimates** are presented.
Time discretization is implemented by decoupling the discrete problem to local systems on the subintervals. However, numerical experiments have shown that the efficient solution of the algebraic system remains challenging, in particular if higher order temporal finite element approaches are involved. We present various preconditioning techniques for GMRES iterations to the local systems. For preconditioning, the **geometric multigrid method with a patchwise Vanka smoother** as well as **blockstructured ILU** based techniques are studied numerically. The preconditioning techniques exploit a tensor product implementation of the STFEMs. The experimental investigations are partly done for the simplified model of acoustic wave propagation.

Multilevel Monte Carlo Simulation of Reactive Transport in Random Porous Media

N. Shegunov, O. Iliev, P. Armyanov

In this work a problem that describes a reactive transport inside a random porous medium is considered. The main driving force of the transport is the processes of convection and diffusion, which are influencing the reaction. This type of simulations has practical applications in oil recovery, soil pollution and remediation, as well as in several industrial and biomedical processes.

A steady-state two-dimensional convection-reaction-diffusion equation with random coefficients is considered. It describes reactive transport in random porous media consisting of sand, gravel, and other soils. The equation is considered in its dimensionless form. The applicability and superiority of MLMC method for solving such problems with a huge parametric space is demonstrated. The coarse grain strategies used for constructing the MLMC model are discussed. Lognormal distribution of the permeability is considered, based on numerous experimental observations. Essential part of the algorithm is the fact that the random coefficients for the flow problem and for the reactive transport are not independent. In fact, random coefficients are generated for the flow problem, and using them coefficients for the reactive transport are derived based on the standard models for flows in porous media and heterogeneous reactions.

Modelling Space-Charge Effects in Resistive Cylindrical Chambers

E. Shumka, P. Petkov, B. Pavlov, A. Petrov, M. Pehlivanova

Resistive Cylindrical Chambers (RCC) have been introduced in recent years as an innovative approach to constructing resistive gaseous detectors. This design offers the advantage of a robust mechanical structure capable of withstanding higher gas pressures, thereby enhancing efficiency. Additionally, the inhomogeneous electric field inherent to this geometry improves avalanche containment, reducing the likelihood of streamers.
Simulating avalanche formation and space-charge effects in RCC is crucial at this stage of their development. These simulations allow for a thorough investigation of the detector's properties and help verify whether the proposed advantages are realized in this novel geometry.
Here, we present a unified interface for conducting all simulation steps using open-source tools. This approach includes enhancements such as parallel execution with MPI and integration of alternative finite-element method (FEM) software, such as FEniCSx, alongside the established Garfield++ simulation package.

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A Wasp-Inspired Model for Adaptive Actor Selection in AI-Driven Stage Visuals

D. Simian, F. Husac

Live performances offer unique opportunities to captivate audiences by blending artistic expression with technological innovation. By introducing advanced tools such as Machine Learning and Generative AI, the visual dimension of performances can be transformed to provide more immersive and emotionally resonant experiences.
In one of our earlier research, we developed an integrated hardware and software framework to enhance live performances by dynamically combining performer visuals with AI-generated backgrounds. Our approach used robotic cameras in a master-slave configuration to track and analyze performers in real time. The master camera processed video data to identify the number of subjects, analyze their facial expressions, and determine emotional states using deep learning techniques. These emotional cues influenced both the selection of a performer for projection and the generation of a tailored visual background. While our prior work introduced sentiment analysis as a key criterion for performer selection, the broader development of a comprehensive selection model and the exploration of additional criteria and scenarios were left as future directions.
In this article, we build on our prior work by introducing a novel targeting model inspired by the adaptive behavior of wasps. This bio-inspired algorithm evaluates multiple dynamic criteria, including emotional analysis, movement patterns, and contribution to the performance, to optimize the selection of performers for projection onto AI-generated visuals. By adapting to real-time changes in multi-actor settings, such as concerts, opera, theater, and choral performances, the proposed model enhances the system's contextual awareness and visual impact. Our proposed model leverages multiple parameters to generate diverse scenarios for performer selection. The article outlines the essential requirements for implementing the model, focusing on its potential to adapt to different performance contexts.

In Silico Analysis of pH Stability in Trypsin-Inhibitor-Based Cyclotide Grafts

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

Peptide aptamers, small proteins capable of binding to variety of target molecules, hold significant potential for modulating or inhibiting these targets. Their binding affinity is closely tied to their conformational flexibility: while flexibility enables adaptation to target surfaces, restricting their conformational ensemble can enhance binding affinity by reducing the entropic contribution. One approach to achieve such conformational

constraint is to graft peptide aptamers onto protein scaffolds, which stabilizes their desired conformation.
Cyclotides, a family of cyclic peptides, are exceptional scaffolds for this purpose due to their remarkable stability and structural diversity. These miniproteins feature a head-to-tail cyclized backbone and a cystine knot motif (CKM) formed by three interlocking disulfide bonds, providing both robustness and adaptability. Grafting involves embedding the peptide aptamer sequence into one of the cyclotide's loop regions without compromising its structural integrity. Successful cyclization and folding of the grafted cyclotides are critical to the production of bioactive molecules that retain the stability and functionality of the cyclotide scaffold.
In this study, we explore the use of molecular modeling to select grafted cyclotides with functional structures. Specifically, we investigate the interactions between the native cyclotide MCoTI-I and its target, trypsin, to understand how binding affects the stability and conformation of the CKM. The goal is to demonstrate that binding to trypsin provides a framework for identifying grafted cyclotide topologies with proper folding and cyclization patterns, paving the way for the development of functional bioactive molecules.

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Practical Application of BURA to Fractional Diffusion Problems with Power Outside of the Unit Interval

D. Slavchev, N. Kosturski, S. Harizanov

Fractional in space derivatives are acknowledged to be essential for the mathematical modelling of fluid dynamics in heterogeneous media and in other physical processes and phenomena. When the fractional parameter α is outside of the unit interval $\alpha \in (0, 1)$, the majority of the numerical methods for efficient approximation of the solution become unsuitable. In this work we investigate the use of repeated BURA approximations with lower power to overcome this difficulty as $\nabla^\alpha = \prod_i \nabla^{\alpha_i}, \alpha > 1, \alpha_i \in (0, 1]$. Here BURA stands for Best Uniform Rational Approximation. We apply optimal normalization of the rational approximation. Based on that, we numerically investigate the benefits of several approaches for the choice of α_i.

Combined Multi-Stage PDE-Based Image Processing: Computational Aspects

K. Slepova, M.B. van Gijzen

Image processing techniques play an important role in tasks such as de- noising, segmentation, and analysis of diverse image datasets. In this paper, we will investigate the computational aspects of a combined multi-stage PDE- based image processing approach. This approach consists of three stages: image formation, noise filtering, relying upon nonlinear diffusion, and image segmentation. These stages can be combined into one nonlinear optimisation problem which is then solved using the alternating direction method of multipliers (ADMM). To evaluate the computational performance and robustness of this approach, we will apply it to a wide range of test images, including both synthetic data and experimental measurements.

On the Optimal Second Order Decrease Rate of a Function for Nonlinear and Symmetric Control Systems

M. Costantini, P. Soravia

When a control system has all its vector fields tangent to the level set of a given smooth function u at a point $\hat{x}$, that function can still have a negative rate of decrease with respect to the trajectories of the control system in appropriate sense if the Lie algebra of the vector fields satisfies appropriate conditions. In the case when the system is symmetric and u has a decrease rate of the second order, we investigate the existence of a best possible rate in the class of piecewise constant controls and the corresponding trajectories. The problem turns out to be purely algebraic, and depends on the eigenvalues of matrices constructed from a basis matrix whose elements are the second order Lie derivatives of u at $\hat{x}$ with respect to the vector fields of the system.

References

[1] J.M. Coron, Control and nonlinearity, Mathematical Surveys and Monographs, 136. American Mathematical Society, Providence, RI, 2007

Sales Forecasting: Combining Regression and Time Series for Adaptive Predictions

J. Stanchov

Sales forecasting is an important task that can provide businesses with the information needed to optimize inventory, plan marketing campaigns and man- age resources. While traditional forecasting models such as linear regression provide powerful analytical tools, they can be limited when trying to predict dynamic and adaptive sales trends. Trends can change quickly and be influ- enced by various external factors such as global events, seasonal campaigns and promotions. Despite its simplicity and interpretability, linear regression has disadvantages, such as a tendency to overfitting when there are many variables or when the variables are highly correlated with each other. Therefore, there is a need to integrate models that can adapt to new data in real time. The ability to forecast in real time allows businesses to make faster and more informed decisions to change marketing campaigns, create new product lines or optimize inventory. Time series methods such as ARIMA and Prophet can capture seasonal and trend dependencies, while LASSO regression offers a way to reduce dimensionality and select important features that influence results. Joint use of LASSO regression with time series models such as ARIMA and Prophet will be explored in this study.

Higher Order Space-time Finite Element Methods for a Poromechanical Model with Memory Effects

J.S. Stokke, M. Bause, N. Margenberg, F.A. Radu

In this talk, we consider a poromechanical model with memory effects, known as the Biot–Allard model. We derive an equivalent formulation where the memory effects are represented by an auxiliary partial differential equation. The system is then rewritten as a first-order system in time and well-posedness is proven using Picard theory. The equations are then discretized by continuous Galerkin methods in time and inf-sup stable pairs of finite element spaces in space. Error estimates are proven and the convergence is studied numerically.

Structural Health Monitoring of Beams by Neural Networks and Supervised Learning

S. Stoykov, E. Manoach

Beams are thin structures that find extensive application in various engineering constructions. Extreme weather conditions and significant deformations frequently cause structural damages to beams. Early identification of damages, accurate localization, and estimation of their magnitude are essential for the effective operation and maintenance of these structures. Inspired by the vibration-based methods and employing a supervised machine learning approach, the current study introduces a structural health monitoring technique for beams. A neural network is designed and trained to detect damage in a beam, localize it, and estimate its magnitude.

Training data for the neural network is generated by numerically solving the equation of motion of the beam. The equation of motion is derived using Timoshenko's beam theory and geometrical type of nonlinearity is included in the model. The resulting partial differential equation is discretized by the finite element method and solved in the time domain by Newmark's time integration scheme. Damage in the beam is modeled by reducing the thickness in the damaged area.

A set of dynamic responses is generated, considering various damages along the beam's length, different excitation forces, and damages of varying magnitudes. Transverse displacements of the beam are stored at multiple instants of time and used to train the neural network. The study demonstrates that the neural network can accurately determine the location and magnitude of the damage. Additionally, the neural network demonstrates high accuracy for time responses with added random noise.

Efficient Preconditioners for Coupled Stokes–Darcy Systems

P. Strohbeck, I. Rybak

In this contribution, we develop and analyse preconditioners for coupled Stokes–Darcy problems and apply them in numerical studies. Such problems are commonly used to model coupled free-flow and porous-medium systems, which play a crucial role in various applications, e.g. industrial filtration, blood flow in the human body, and surface/subsurface flow interactions.
The Stokes equations describe fluid flow in the free-flow domain, while Darcy's law is applied in the porous medium. The two sets of equations are coupled by suitable interface conditions at the fluid–porous interface. In this work, we consider different types of coupling concepts.
Discretising coupled Stokes–Darcy problems yields linear systems, where the matrix is large, sparse, ill-conditioned, and often non-symmetric. While the majority of existing literature uses finite element methods, we consider a second-order finite volume method for discretisation as this approach ensures mass conservation, stability, and natural coupling across the fluid–porous interface. The resulting linear systems require efficient and robust preconditioners to accelerate the convergence of iterative solvers. Therefore, we develop several novel preconditioners. We conduct spectral analysis of the preconditioned systems to show the enhanced convergence of the iterative method. Since direct use of the exact preconditioners is computationally expensive, we also present efficient inexact versions. The efficiency and robustness of the preconditioners is demonstrated in several numerical examples.

Domain Decomposition-based Coupling of Intrusive and Non-intrusive Reduced Order Models via the Schwarz Alternating Method

I. Tezaur, C. Wentland, I. Moore, E. Parish, A. Gruber, A. Mota

This talk will describe a novel domain decomposition-based approach for creating adaptive hybrid models with the help of the Schwarz alternating method (SAM). In this approach, the solution on the full domain is obtained via an iterative process in which a sequence of subdomain-local problems are solved, with information propagating between subdomains through transmission boundary conditions (BCs). The models being coupled can be subdomain-local full order models (FOMs) and/or subdomain-local intrusive or non-intrusive reduced order models (ROMs). We will present some recent extensions of SAM to enable the coupling of subdomain-local non-intrusive ROMs constructed via Operator Inference (OpInf). We will show numerical results that demonstrate the method's performance on several benchmarks. We will additionally discuss some perspectives towards enabling on-the-fly switching between subdomain-local models of varying fidelities within the SAM framework.

Analysis of the Contribution of Thrombophilia Polymorphisms to Early Onset Miscarriages

T. Tiankov, E. Abadjieva, R. Comsa, I. Dimova, A. Savov, S. Todinova, S. Krumova, A. Alexandrova, I. Tsakovska, T. Pencheva

One of the most common complications that can occur during pregnancy is pregnancy loss, accounting for approximately 20% of pregnancy abnormalities, nearly 18% of which are recurrent miscarriages.

Increased procoagulant activity during pregnancy is a prerequisite for triggering thrombotic events. These in turn can lead to placental hypercoagulability and microthrombosis, which may result in recurrent miscarriages in the first trimester. Although the etiology of early pregnancy loss is not fully understood, genetic predisposition is believed to be a contributing factor. The presence of multiple risk factors further increases the likelihood of pregnancy complications. Understanding the genetic basis of such events requires integrating vast amounts of data from genomics and other biomedical data sources and their thorough analysis by the application of advanced mathematical and computational approaches.

For the statistical analysis of such data, a web application was developed on Django – a high-level Python web framework. Python SQLite3 module is used to integrate the SQLite database with Python. The application allows for the automatic finding of the absolute frequency of the most frequently studied thrombophilia factors, e.g. factor V Leiden (FVL) mutation, mutation FII20210G>A in the prothrombin gene, polymorphism C677T in the methylenetetrahydrofolate reductase (MTHFR) gene, and 4G/5G polymorphism in the PAI-1 gene, on large datasets generated for women with miscarriages. The frequency of the presence of two or more mutations simultaneously for a certain age category and/or for a certain number of spontaneous abortions can be determined.

Our results demonstrate that the carrier of MTHFR significantly contributes to recurrent miscarriages, followed by 4G/5G polymorphism in the PAI-1 gene, while carriage of FVL and FII20210G>A in the prothrombin gene is of lesser importance to recurrent miscarriages specifically in Bulgaria.

The presented results provide important insights into the genetic factors that should be of priority interest for future research and clinical screening in women with recurrent miscarriages and can serve as a basis to develop predictive models for assessing the risk of spontaneous abortion in individuals based on their genetic status. The findings on MTHFR and PAI-1 polymorphisms suggest that interventions to address folate metabolism or fibrinolysis may be particularly useful in preventing miscarriage in women with such genetic predispositions.

New Kirkman Triple Systems of Order 45

S. Topalova, S. Zhelezova

Let $V = \{P_i\}_{i=1}^{v}$ be a finite set of points, and $\mathcal{B} = \{B_j\}_{j=1}^{b}$ a finite collection of k-element

subsets of V called blocks. If any 2-element subset of V is contained in exactly λ blocks of $\mathcal{B}$, then $D = (V, \mathcal{B})$ is a 2-(v, k, λ) design. A 2-$(v, 3, 1)$ design is a Steiner Triple Systems of order v (STS(v)). An STS(v) is cyclic if it possesses an automorphism group which permutes its points in one cycle of length v. There is a one-to-one correspondence between cyclic STS(v)s and $(v, k, 1)$ cyclic difference families. All cyclic STS(45)s are 11616 and were classified in 1994.
A parallel class is a partition of the point set V by blocks of $\mathcal{B}$. A resolution of an STS(v) is a partition of the collection of blocks to parallel classes. An STS(v) together with a resolution of its blocks is called a Kirkman triple system (KTS(v)). KTS(v)s exist iff $v \equiv 3 (\text{mod } 6)$, $v \geq 3$. KTS(v)s have numerous applications and are therefore subject of intensive research. They are completely classified up to order 15. The known KTS(v)s of bigger orders have been constructed with prescribed automorphisms or with subsystems. A KTS(v) is point-cyclic if the resolution parallel classes are preserved by a cyclic automorphism group of order v. Recently all point-cyclic resolutions were classified for $v \in \{45, 57\}$. In the present work we construct resolutions of the cyclic STS(45)s invariant under the subgroup of order 15 of the cyclic automorphism group of order 45. This is a difficult task because the number of parallel classes invariant under a particular automorphism group grows rapidly as the group order decreases. We succeed to solve this problem using the High-performance computing system Avitohol. We also establish if the constructed KTS(45)s possess some additional properties which are important for possible applications to different kinds of LDPC codes and erasure-resilient codes for large disk arrays.

Policies to Curtail the Size of the Informal Sector in an Economy with Fiscal Rules

T. Tsachev, I. Vassileva

To explore various policies for curbing the informal sector we build a dynamic general equilibrium model with two sectors (official and informal), two households (skilled and unskilled) and a government, guided by fiscal rules. The assumptions of the model allow us to to consider the skilled household and the official production sector as one decision maker, the same is valid for the unskilled household and the informal production sector. The model is calibrated to the Bulgarian economy. In this setting we compare two policy options: a reduction of the tax rate on personal income and social security contributions and enhanced efforts of the tax administration to detect informal activities. Furthermore, we study the properties of the model and prove that both the skilled and unskilled households problems have unique interior solutions.

Efficient Monte Carlo Solutions for High-Dimensional Fredholm Integral Equations

V. Todorov, S. Apostolov, P. Zhivkov, S. Fidanova, I. Dimov

Integral equations are fundamental tools in many areas of applied mathematics, physics, and engineering. They find widespread application in disciplines such as mechanics, geophysics, the kinetic theory of gases, quantum mechanics, mathematical economics, and queuing theory, among others. The diverse applications of these equations demand the development of efficient, robust, and flexible solution techniques. This study introduces an unbiased stochastic method for solving multidimensional Fredholm integral equations of the second kind. The approach is tailored to deliver high precision while keeping computational demands low, making it well-suited for tackling complex problems with irregular kernels and solutions.

A key feature of the approach is its unbiased estimation, which ensures that the computed solution does not systematically deviate from the true solution, even in high-dimensional settings. This property is achieved by rigorously balancing the sampling strategy with the properties of the Fredholm kernels and the integration domains. The method demonstrates robust convergence properties under a wide range of conditions, including complex, non-separable kernels and irregular integration domains.

Extensive numerical experiments are conducted to validate the performance of the method, comparing it against state-of-the-art deterministic and biased stochastic solvers. Results show that the proposed unbiased Monte Carlo approach achieves superior scalability and accuracy, particularly for problems with dimensions exceeding five, where traditional methods often fail due to computational intractability. This work underscores the importance of unbiased stochastic methods as a viable and powerful alternative for solving high-dimensional Fredholm integral equations, paving the way for their broader application in scientific and industrial problem-solving.

Intelligent Simulation-Based European Option Valuation

V. Todorov, B. Chakarov, S. Hadzhiivanov, M. Chechev, Y. Dimitrov

Multidimensional options, also known as multi-asset options, are financial derivatives whose value depends on the performance of multiple underlying assets. These instruments have gained significant popularity due to their ability to address complex financial strategies, such as portfolio diversification, spread trading, and correlation hedging. However, pricing and hedging multidimensional options present formidable computational challenges due to their high dimensionality and intricate payoff structures.

Valuing multi-dimensional options remains a critical challenge in modern large-scale financial applications. A European call option provides the holder with the right, but not the obligation, to acquire a specific underlying asset S at a predetermined strike price K on or before a specified maturity date T. Monte Carlo and quasi-Monte Carlo techniques have become indispensable for addressing a wide range of financial problems. This study

emphasizes the accurate numerical evaluation of multi-dimensional European options, leveraging the strength of Monte Carlo approaches, particularly in high-dimensional settings. We introduce optimization techniques based on low-discrepancy sequences and variance reduction methods, achieving substantial improvements in accuracy compared to traditional approaches. This enhanced precision is essential for reliable option pricing and is particularly advantageous in cases where deterministic methods fall short, such as in high-dimensional contexts or when dealing with complex contractual structures.

Refined Stochastic Methods for Large Linear Algebraic Systems

V. Todorov, V. Traneva, S. Tranev, Y. Dimitrov, S. Apostolov

Solving large-scale algebraic systems efficiently and accurately remains a central challenge in computational science and engineering. Traditional deterministic methods, such as direct solvers or iterative schemes, often face difficulties in scalability, convergence, and computational cost when applied to systems with high dimensionality or complex structures. This paper introduces Refined Stochastic Methods—a suite of advanced stochastic techniques designed to tackle large algebraic systems with improved efficiency, accuracy, and robustness.
The cornerstone of this research is the development of Monte Carlo "walk on equations" algorithms and their enhanced variants, tailored specifically for linear algebraic systems. These methods leverage probabilistic sampling to estimate solutions, making them particularly suitable for systems arising from high-dimensional problems or involving sparse and ill-conditioned matrices. Unlike deterministic approaches, stochastic methods exhibit inherent flexibility in handling systems with irregular structures or incomplete information.
In conclusion, the refined stochastic methods presented in this paper provide a robust and scalable alternative for solving large algebraic systems, offering a powerful toolset for applications in science, engineering, and data-driven fields. The proposed techniques pave the way for future research into advanced stochastic methods and their integration with emerging computational paradigms, such as parallel and quantum computing.

A Circular Intuitionistic Fuzzy Approach to the Zero Point Transportation Problem

V. Traneva, S. Tranev

Transportation problems (TPs) are crucial for optimizing the management of transport deliveries. In classical TPs, decision-makers typically assume precise values for transportation costs, supply, and demand. However, real-world parameters often involve ambiguity and vagueness due to uncontrollable factors such as economic instability, fluctuating fuel prices, road conditions, and weather. To address these challenges, Atanassov

introduced the Circular Intuitionistic Fuzzy Set (C-IFS) in 2020, an extension of the Intuitionistic Fuzzy Set, to better model environmental uncertainty.
This paper presents a novel circular intuitionistic fuzzy zero-point approach to transportation problems under the Circular Intuitionistic Fuzzy Transportation Problem (C-IFTP) framework. The proposed method evaluates transportation costs, supply, and demand values using expert-assigned circular intuitionistic fuzzy numbers. An optimal solution algorithm is developed based on the index matrix concept, incorporating additional constraints such as transportation cost limits.
The efficiency of the C-IFTP algorithm is demonstrated through a case study involving a humanitarian organization optimizing the transportation of essential supplies from warehouses to disaster-affected regions. The study evaluates three decision-making scenarios: pessimistic, optimistic, and average.
The originality of this work lies in the definition of the C-IFTP framework and its application to solving transportation problems with imprecise parameters. This approach provides a robust and adaptable solution for decision-makers facing uncertainty and can be extended to address other types of C-IFT problems.

Intuitionistic Fuzzy Monte Carlo Simulations for Environmental Sensitivity Analysis under Multidimensional Uncertainty

V. Traneva, S. Tranev, S. Georgiev, V. Todorov

This study presents a novel framework integrating intuitionistic fuzzy logic with Monte Carlo simulations to enhance multidimensional sensitivity analysis in the Unified Danish Eulerian Model (UNI-DEM), a key tool for modeling the long-range transport of air pollutants. Traditional Monte Carlo methods often rely on precise input data, limiting their utility when inputs—such as emission rates, chemical reaction constants, and boundary conditions—are uncertain or imprecise. To overcome this limitation, we propose an intuitionistic fuzzy Monte Carlo approach that utilizes intuitionistic fuzzy numbers to model input uncertainties and propagates them through the system using intuitionistic fuzzy arithmetic and stochastic sampling techniques.
The framework extends conventional sensitivity analysis by incorporating fuzzy Sobol indices, allowing for a detailed quantification of parameter contributions to model output variability under uncertain conditions. Validation is performed through case studies involving major European cities, highlighting the impact of uncertainties in anthropogenic emissions and chemical reaction rates on pollutant concentrations. Comparative analyses with traditional and quasi-Monte Carlo methods underscore the robustness and computational efficiency of the proposed approach.
The findings emphasize the critical importance of accounting for input uncertainties in sensitivity analyses, offering policymakers a more reliable foundation for environmental decision-making. By bridging intuitionistic fuzzy logic with advanced stochastic techniques, this research represents a significant advancement in environmental modeling and uncertainty quantification.

Interpolation Spaces, Fractional Order Operators, and Scales of Multilevel Decompositions

P.S. Vassilevski

In applications involving Monte Carlo simulations for computing QoI (quantities of interest) based on solving PDEs with stochastic coefficients, one needs efficient ways to sample these coefficients from certain distributions. The sampling process itself can be formulated as solving an elliptic PDE with a random r.h.s. (so-called white noise). There is a scale of PDEs that produce random coefficients from a scale of distributions. In this presentation, we will provide an application of the interpolation theory of spaces and operators to define such scales. Secondly, in the finite element setting, we will consider computationally feasible alternatives involving computable hierarchical decomposition of fractional order operators. Some theoretical results as well as numerical illustrations will be presented.

Revisiting Composite Adaptive AMG

P.S. Vassilevski

The adaptive algebraic mutigrid methods (aAMG), also known as bootstrap AMG, are constructed recursively by testing the convergence of the current method available at a given stage on the homogeneous equation starting with a nonzero (random) guess. By doing so, we are able to detect error components that the current method cannot annihilate. The detected error component is then incorporated to build an improved solver. One approach that we investigate is to use the newly detected error component, commonly referred as to *algebraically* smooth vector, to guide the construction of a new AMG hierarchy and respective AMG solver. By composing the new AMG solver with the previous method we end up with the so called composite adaptive AMG methods. We can see the analogy between the composite aAMG and a Krylov iterative method; namely, in the former at every adaptation step we generate a new algebraically smooth vector and respective AMG solver guided by that vector, whereas in Krylov methods at every new step we generate a new search direction and augment the Krylov space which results, in both cases, in improved convergence, with the expectation that they would require much less that n steps (n being the problem size).
In this presentation, we discuss some recent theoretical and algorithmic developments in this area.

Parallel Algorithm for Solving Dipolar Gross-Pitaevskii Equation

D. Vudragović, V. Lončar, A. Balaž

From a theoretical standpoint, Bose-Einstein condensates (BEC) are generally analyzed using the framework of second quantization. The corresponding many-body Hamiltonian includes two types of particle interactions: short-range contact interactions and long-range dipole-dipole interactions. Because these interactions are typically weak, they can be addressed using perturbation theory, which enables a basic description of the system through mean-field theory.

At zero temperature, thermal excitations can be neglected, allowing us to apply mean-field theory, which leads to the Gross-Pitaevskii equation (GPE). In systems where dipole interactions are present, the standard GPE needs to be modified to include the relevant dipolar interaction terms. These modified equations are often referred to as nonlinear Schrödinger equations due to the presence of terms resulting from nonlinear interactions. They can accurately describe nearly all phenomena observed in BEC systems.

There are several numerical methods available for solving the dipolar GPE, which include analyzing both the ground state properties and the non-stationary dynamics of a BEC. These methods can be categorized into three main types: finite difference, split-step, and spectral methods. In this talk, we present our numerical algorithm for solving the GPE, which combines the split-step method with the semi-implicit Crank-Nicolson approach. To calculate the ground state of the system, we use imaginary time propagation starting from an arbitrary initial state. In contrast, the dynamics of the system are determined through real-time propagation from a given initial wave function. We also present various parallelization strategies, aimed at both shared memory and distributed memory systems, with a particular focus on heterogeneous computing platforms.

Parallel Adaptive Simulation of Processes from Science and Engineering

G. Wittum

Numerical simulation has become one of the major topics in Computational Science. To promote modelling and simulation of complex problems new strategies are needed allowing for the solution of large, complex model systems. Crucial issues for such strategies are reliability, efficiency, robustness, usability, and versatility.

After discussing the needs of large-scale simulation we point out basic simulation strategies such as adaptivity, parallelism and multi-grid solvers. To allow adaptive, parallel computations the load balancing problem for dynamically changing grids has to be solved efficiently by fast heuristics. These strategies are combined in the simulation system UG ("Unstructured Grids") being presented in the following.

In the second part of the seminar we show the performance and efficiency of this strategy in various applications. In particular, the application and benefit of parallel adaptive multi-grid methods to modelling drug permeation through human skin is shown in detail.

Numerical Simulation of Phase Transitions for Saline Groundwater Flow in Soils with Permafrost

R. Wittum, A. Nägel, D. Logashenko, G. Wittum

In determining suitable locations for the long-term storage of nuclear waste, simulations of groundwater flow based on real geological data are indispensable. Accurate prediction of the groundwater flow for future decades and millennia raises significant challenges for mathematical modelling, numerical methods and software implementation. One of the main concerns is handling of permafrost soils which might form by freezing ground or recede through melting during the period of interest. It has a principal impact on the flow patterns. A further important aspect is the density-driven flow arising for example due to the dilution of the saline groundwater by the melt water from the permafrost.
The purpose of this work is extension of the existing freeze-thaw model in porous media with salinity and developing efficient numerical methods for it. We propose a fully coupled system of partial differential equations describing the density-driven groundwater flow with the phase transitions due to the freeze-thaw phenomena. For this model, we present a collocated vertex-based finite volume discretization and a linearly implicit time stepping scheme (LIMEX). Application of this time discretization allows to catch automatically the correct time scales of the flow and phase transition processes. To achieve high spatial resolution, we apply an efficient linear solver based on the geometric multigrid preconditioner. Our implementation is based on the ug4 simulation toolbox.
For our numerical experiments, we implemented and expanded the INTERFROST benchmark. We demonstrate the effect of salinity and show that considering freezing point depression depending on salt mass fraction leads to a faster melting process in saline soils.

Quantum Machine Learning for Structure-Based Virtual Screening

P.-K. Yang, J.-H. Lin

It has been estimated by graph theory that there are at least 10^{60} small organic molecules in the biologically relevant chemical space for drug discovery. An essential component in the structure-based virtual screening for lead candidates is the accurate estimation of the binding free energy between the small organic molecule and its target protein. Even with the rather inexpensive machine learned methods to estimate the binding free energies for screening against a typical ultra-large chemical library of about 10^8 chemical molecules can already take quite a significant amount of computational resources, not to mention to explore the chemical space of about 10^{60} molecules. Universal gate-based quantum computers hold the promise to explore the entire space of medicinal chemistry in the future. In this work, we show how we implemented a quantum machine learning approach with quantum circuits to evaluate the binding free energies between small molecules and their target proteins in the protein-ligand complex structures simultaneously. We used the structural files of protein-ligand complexes and experimental pK_D values curated in PDBbind v2020, which consists of the so-called "general" set of 14,127 protein-ligand complexes and the so-called "refined set" of 5,316 protein-ligand complexes. We then converted the coordinates and atom types of the protein-ligand complexes into 512 so-called "occupancies", and designed a quantum circuit to optimize the values of the parameters. We used additional nine qubits for evaluating the binding free energies (ΔG_{bind}) of protein-ligand complexes. With 1440 parameters to prepare the classical occupancies and then the quantum states describing the structures of the protein-ligand complexes, and 45 parameters to predict the binding free energies (ΔG_{bind}), the Pearson correlation coefficient (PCC) between the estimated binding free energies and their original experimental binding fre energies can be as high as 0.78, and the root mean square error (RMSE) is as low as 1.59 kcal/mol. Our work demonstrated that effective evaluation of protein-ligand binding free energy can be implemented with univeral gate-based quantum computers.

A Multipoint Stress-Flux Mixed Finite Element Method for the Biot System of Poroelasticity on Distorted Quadrilateral Grids

I. Yazici, I. Yotov

We present a mixed finite element method for a five-field formulation of the Biot system of poroelasticity, which reduces to a cell-centered pressure-displacement system on distorted quadrilateral grids. The method couples a mixed stress-displacement-rotation formulation for elasticity with weak stress symmetry and a mixed velocity-pressure Darcy formulation. The spatial discretization combines the multipoint stress mixed finite element method for elasticity with the multipoint flux mixed finite element method for Darcy flow. The method employs the lowest-order Brezzi-Douglas-Marini mixed finite element space for the poroelastic stress and Darcy velocity, piecewise constant displacement and pressure, and continuous piecewise bilinear rotation. Symmetric and non-symmetric vertex quadrature rules are applied to the velocity, stress, and stress-rotation bilinear forms, block-diagonalizing the corresponding matrices and allowing for local elimination of velocity, stress, and rotation. This leads to a cell-centered positive-definite system for pressure and displacement at each time step. We conduct stability and error analysis for the fully discrete formulation, establishing first-order convergence for all variables in the L2-norm. Numerical tests illustrate the theoretical convergence rates.

Adaptive Nonoverlapping Preconditioners for the Helmholtz Equation

Y. Yu, M. Sarkis, G. Li, Z. Zhang

One of the issues with traditional preconditioning of the Helmholtz equations is the potential ill-posedness of the local Dirichlet boundary problem. In this talk, we introduce a new iterative substructuring method, which is similar in concept to the Schur complement system used for elliptic problems. This new structure ensures the well-posedness of the local Dirichlet problems by incorporating the small-magnitude eigenvalues from each subdomain into the coarse problem. Another key challenge of traditional preconditioning of the Helmholtz equations lies in constructing an effective coarse space for non-overlapping methods. Motivated by the success of using generalized eigenvalue problems to precondition elliptic equations with heterogeneous coefficients, we propose two types of DDMs that construct a robust coarse problem. Moreover, our construction is purely algebraic, facilitating straightforward extension to other discretizations and the case of heterogeneous Helmholtz coefficients, while convergence theorems remain valid when the thresholds are close to one.

A Space-Time Continuous Galerkin Finite Element Method for Linear Schrödinger Equations

M. Zank

Classical approaches of full discretization schemes of time-dependent partial differential equations are based on explicit or implicit time-stepping schemes connected with finite element methods in space. Space-time methods, i.e., the temporal variable t is just another spatial variable, are an alternative. In this case, the space-time domain Q is subdivided by using a space-time mesh, and the resulting global linear system has to be solved at once.

In this talk, the model problem is the linear time-dependent Schrödinger equation with homogeneous Dirichlet boundary conditions. As a full approximation scheme, we focus on the design of a space-time continuous Galerkin finite element method. For this purpose, we introduce a space-time variational formulation of the Schrödinger equation in $H^1(Q)$. We analyze the unique solvability of this variational setting. Next, a space-time discretization scheme based on piecewise polynomial, globally continuous trial and test functions is considered. In particular, we examine a tensor-product approach, including stability and related CFL conditions. In the last part of the talk, we show numerical examples.

Sensitivity Analysis of Volume Spread Analysis-Based Trading Algorithms Using Monte Carlo Simulation

P. Zhivkov, V. Todorov

The success of algorithmic trading strategies, like those based on Volume Spread Analysis (VSA), largely depends on how well their parameters are set. Sensitivity analysis is good for understanding how changes in these parameters influence performance.
This study explores the application of Monte Carlo simulation as an ap- proach to conducting sensitivity analysis for VSA-based trading algorithms. Monte Carlo methods will facilitate a comprehensive evaluation of the algo- rithm's behaviour across a wide range of market conditions. These param- eters are modified within predetermined ranges to determine their impact on important performance indicators such as profitability, drawdown, and risk-adjusted returns (for example, Sharpe ratio).
The model uses a rolling window of 168 candles and adjusts continuously to recent market conditions, using volume as the independent variable and price spread as the dependent variable. This dynamic framework allows for real-time adjustments and generates a baseline "expected" spread for each new data point. The difference between actual and predicted spread values is treated as an indicator: a positive deviation suggests an unexpectedly wide price range given the current volume, while a negative deviation suggests a narrow price range despite substantial trading volume.
Preliminary results from the Monte Carlo simulation show modifying stop-loss thresholds between 5% and 15% revealed a 20% variance in aver- age profitability, with more aggressive thresholds (e.g.,5%) leading to higher returns but also increased drawdowns.
The study shows the advantages of Monte Carlo simulation in uncovering parameter sensitivities that might otherwise go unnoticed in deterministic or other analyses. By integrating sensitivity analysis into the development pipeline, trading algorithm developers can enhance the adaptability of their systems across varying market fluctuations.

On Discretizations Using Quasi-polynomial Spaces of Differential Forms

L.T. Zikatanov

We consider quasi-polynomial spaces of differential forms defined as weighted (with a positive weight) spaces of differential forms with polynomial coefficients. We show that the unisolvent set of functionals for such spaces on a simplex in any spatial dimension is the same as the set of such functionals used for the polynomial spaces. The analysis in the quasi-polynomial spaces, however, is not standard and requires a novel approach. We are able to prove our results without the use of Stokes' Theorem, which is the standard tool in showing the unisolvence of functionals in polynomial spaces of differential forms. These new results provide tools for studying exponentially-fitted discretizations stable for general convection-diffusion problems in Hilbert differential complexes.

This is a joint work with Shuonan Wu (Beijing University) and extension of a joint work with Raytcho Lazarov (2005 Obchysljuval'na ta prykladna matematyka, Kiev).

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