13th International Conference
June 7 - 11, 2021
Sozopol, Bulgaria

LARGE-SCALE SCIENTIFIC COMPUTATIONS LSSC'21

Scientific Program
Abstracts
List of Participants

IICT
Institute of Information and Communication Technologies
Bulgarian Academy of Sciences
1869

PREFACE

The thirteenth International Conference on "Large-Scale Scientific Computations" LSSC 2021 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:

Yalchin Efendiev, (Texas A&M University, College Station, TX, US)
Xiaozhe Hu, (Tufts University, MA, US)
Oleg Iliev, (ITWM, Kaiserslautern, DE)
Mario Ohlberger, (University of Münster, DE)
Yuri Vassilevski, (Marchuk Institute of Numerical Mathematics, RAS, Moscow, Russia)

LIST OF SPECIAL SESSIONS:

- Fractional Diffusion Problems: Numerical Methods, Algorithms and Applications
  organized by Stanislav Harizanov (IICT-BAS, BG), Raytcho Lazarov (TA&MU, College Station, US), HongGuang Sun (Hohai University, Nanjing, CN), Zhi Zhou (Hong Kong Polytechnic University, HK), Petr Vabishchevich (Nuclear Safety Institute, Russian Academy of Sciences, RU)

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

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

- Robust Iterative Solution Methods for Coupled Problems in Poromechanics
  organized by Johannes Kraus (University of Duisburg-Essen, DE), Maria Lymbery (University of Duisburg-Essen, DE)

- Advanced Discretizations and Solvers for Coupled Systems of Partial Differential Equations
  organized by James Adler (Tufts University, US), Xiaozhe Hu (Tufts University, US), Raytcho Lazarov (TA&MU, College Station, US), Ludmil Zikatanov (Pennsylvania State University, US)

- Optimal Control of ODEs, PDEs and Applications
  organized by Michele Palladino (GSSI, L'Aquila, IT), Teresa Scarinci (University of L'Aquila, IT)
- Tensor and Matrix Factorization for Big-Data Analysis
  organized by Boian Alexandrov (Los Alamos National Laboratory, US), Hristo Djidjev (Los Alamos National Laboratory, US)
- Machine Learning and Model Order Reduction for Large Scale Predictive Simulations
  organized by Oleg Iliev (ITWM, Kaiserslautern, DE), Mario Ohlberger (University of Münster, DE)
- HPC and Big Data: Algorithms and Applications
  organized by Aneta Karaivanova (IICT-BAS, BG), Todor Gurov (IICT-BAS, BG), Emanouil Atanassov (IICT-BAS, BG)

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

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11:35 - 12:00	N. Magino, H. Andrä, F. Welschinger, R. Müller, M. Schneider, A Multiscale Approach to Fatigue-Damage Modeling In Short-Fiber Reinforced Plastics, p. 60
	Lunch Break

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Chairperson	S. Fidanova
09:00 - 09:25	S. FIDANOVA, O. Roeva, Influence of the ACO Evaporation Parameter for Unstructured Workforce Planning Problem, p. 40
09:25 - 09:50	P. ZHIVKOV, A. Simidchiev, Quantitative Relationship Between High Concentrations of Particulate Matter and Morbidity, p. 80
09:50 - 10:15	A. Bădică, C. BĂDICĂ, I. Buligiu, L. Ciora, D. Logofătu, Optimal Knock-Out Tournaments: Definition and Computation, p. 28
	Coffee Break
10:45 - 12:00	*Special Session on "Application of Metaheuristics to Large-Scale Problems"*
Chairperson	S. Fidanova
10:45 - 11:10	A. Alihodzic, M. CHAHIN, New Clustering Techniques of Node Embeddings Based on Metaheuristic Optimization Algorithm, p. 24
11:10 - 11:35	A. ALIHODZIC, E. Zvornicanin, A Comparison of Machine Learning Methods for Forecasting Dow Jones Stock Index, p. 24
11:35 - 12:00	K. PENEV, Synergy between Convergence and Divergence - Review of Concepts and Methods, p. 67
	Lunch Break

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Chairperson	G. Colombo
14:00 - 14:25	A. Marigonda, Random Lift of Set-Valued Maps and Applications, p. 61
14:25 - 14:50	G. Cavagnari, Evolution Equations in Wasserstein Spaces Ruled by Probability Vector Fields, p. 36
14:50 - 15:15	A. Lai, M. Motta, Stabilizability in Optimization Problems, p. 57
	Coffee Break
16:10 - 18:15	*Special Session on "Robust Iterative Solution Methods for Coupled Problems in Poromechanics"*
Chairperson	J. Kraus
16:10 - 16:35	F. Radu, Efficient solvers for Poromechanics, p. 69
16:35 - 17:00	J. Both, J. Nordbotten, F. A. Radu, J. M. Sargado, E. Storvik, An Accelerated Staggered Scheme for Phase-field Models of Hydraulic Fracture in Poroelastic Media, p. 32
17:00 - 17:25	Y. Li, L. Zikatanov, Space-Time Error Indicator for Biot's Consolidation Model, p. 58
17:25 - 17:50	J. Adler, Monolithic Multigrid for a Reduced-Quadrature Discretization of Poroelasticity, p. 23
17:50 - 18:15	J. Brannick, Bootstrap AMG, p. 33

Tuesday, June 8

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14:00 - 15:15	*Special Session on "Advanced Discretizations and Solvers for Coupled Systems of Partial Differential Equations"*
Chairperson	L. Zikatanov
14:00 - 14:25	P. Vabishchevich, Decoupling Methods for Systems of Parabolic Equations, p. 76
14:25 - 14:50	S.-Y. Yi, S. Lee, L. Zikatanov, Locking Free and Locally Conservative Enriched Galerkin Methods for Poroelasticity, p. 78
14:50 - 15:15	A. Budisa, X. Hu, M. Kuchta, K.-A. Mardal, L. Zikatanov, Interface Preconditioners for Multiphysics Problems, p. 34
	Coffee Break
16:10 - 17:50	*Special Session on "Advanced Discretizations and Solvers for Coupled Systems of Partial Differential Equations"*
Chairperson	J. Adler
16:10 - 16:35	J. Adler, C. Cavanaugh, X. Hu, L. Zikatanov, A Finite-element Framework for a Mimetic Finite-difference Discretization of Maxwells Equations, p. 23
16:35 - 17:00	X. Hu, K. Wu, L. Zikatanov, A Posteriori Error Estimates for Solving Graph Laplacians, p. 48
17:00 - 17:25	A. Pe de la Riva, F. Gaspar, C. Rodrigo, Isogeometric Analysis for Poroelasticity, p. 38
17:25 - 17:50	J.-L. Guermond, B. Popov, B. Clayton, Invariant Domain Preserving Approximations for the Euler Equations with a Tabulated Equation of State, p. 46

Tuesday, June 8

Parallel Sessions
Lecture Hall C

14:00 - 14:50	*Contributed Talks*
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14:00 - 14:25	H. Gfrerer, J. Outrata, J. Valdman, The Semismooth Newton Method for the Solution of Contact Problems with Tresca Friction, p. 44
14:25 - 14:50	C. Matonoha, A. Moskovka, J. Valdman, Minimization of Energy Functionals via the Finite Element Method in MATLAB, p. 61
	Coffee Break
16:10 - 18:40	*Special Session on "Tensor and Matrix Factorization for Big-Data Analysis"*
Chairperson	B. Alexandrov
16:10 - 16:35	V. Stanev, B. Aleksandrov, Nonnegative Matrix and Tensor Factorizations in the Analysis of Scientific Text Documents, p. 72
16:35 - 17:00	G. Manzini, A Nonnegative Tensor-train Based Method for the Smoluchowski Coagulation Equation, p. 60
17:00 - 17:25	P. Georgiev, Tensor Networks of Sparse Non-Negative Tensors, p. 43
17:25 - 17:50	M. Ishteva, P. Dreesen, Solving Systems of Polynomial Equations a Tensor Approach, p. 51
17:50 - 18:15	E. Pelofske, G. Hahn, D. O'Malley, H. Djidjev, B. Alexandrov, Boolean Hierarchical Tucker Networks on Quantum Annealers, p. 66
18:15 - 18:40	E. Robeva, Exact and Efficient Structured Tensor Decomposition, p. 70

Wednesday, June 9

Parallel Sessions
Lecture Hall A

09:25 - 10:15 *Special Session on "Robust Iterative Solution Methods for Coupled Problems in Poromechanics"*

Chairperson J. Kraus

09:25 - 09:50 K. Osthues, A New Family of Hybridized Discontinuous Galerkin/hybrid Mixed Discretizations for Multiple Network Poroelasticity, p. 64

09:50 - 10:15 J. Kraus, M. Lymbery, F. Philo, On the Stability of Time-discrete Systems Arising from Second-order Implicit Time-stepping Schemes Applied to Dynamic Multiple Network Poroelasticity Models, p. 56

Coffee Break

10:45 - 12:00 *Contributed Talks*

Chairperson I. Lirkov

10:45 - 11:10 S. Georgiev, L. Vulkov, Recovering the Time-Dependent Volatility in Jump-Diffusion Models from Pointwise and Nonlocal Price Observations, p. 43

11:10 - 11:35 K. Jain, Extreme Scale Computations of Transitional Regime in Physiologic Flows, p. 52

11:35 - 12:00 M. Koleva, L. Vulkov, Fitted Finite Volume Method for an Unsaturated Flow Problem with Space Degeneration, p. 54

Lunch Break

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Parallel Sessions
Lecture Hall B

09:00 - 10:15	*Special Session on "Large-Scale Models: Numerical Methods, Parallel Computations and Applications"*
Chairperson	K. Georgiev
09:00 - 09:25	O. Axelsson, D. Lukas, M. Neytcheva, An Exact and Approximate Schur Complement Method for Time-harmonic Optimal Control Problems, p. 28
09:25 - 09:50	Z. Zlatev, I. Dimov, I. Faragó, K. Georgiev, Á. Havasi, Running Atmospheric Chemistry Module of a Large Air Pollution Model by Using Advanced Versions of the Richardson Extrapolation, p. 80
09:50 - 10:15	P. D'Ambra, F. Durastante, S. Filippone, Scalable Preconditioners for Computational Science at Extreme Scale, p. 37
	Coffee Break
10:45 - 11:35	*Special Session on "Large-Scale Models: Numerical Methods, Parallel Computations and Applications"*
Chairperson	M. Neytcheva
10:45 - 11:10	T. Bayleyegn, I. Farago, A. Havasi, On the Consistency Order of Runge-Kutta Methods Combined with Active Richardson Extrapolation, p. 29
11:10 - 11:35	S. Korotov, On Red Refinements of Tetrahedral Meshes, p. 54

Lunch Break

14:00-17:00 *EXCURSION*

Thursday, June 10

Parallel Sessions
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09:00 - 10:15	Contributed Talks
Chairperson	T. Ostromsky
09:00 - 09:25	F. Benkhaldoun, A. Bradji, T. Ghoudi, A Finite Volume Scheme for a Wave Equation with Several Time Independent Delays, p. 31
09:25 - 09:50	P. Popov, V. Iliev, G. Fitnev, Quality Optimization of Seismic-derived Surface Meshes of Geological Bodies, p. 68
09:50 - 10:15	F. Benkhaldoun, A. Bradji, A New Error Estimate for a Primal-Dual Crank Nicolson Mixed Finite Element Using Lowest Degree Raviart Thomas Spaces for Parabolic Equations, p. 30
	Coffee Break
10:45 - 12:00	*Special Session on "Optimal Control of ODEs, PDEs and Applications"*
Chairperson	A. Dontchev
10:45 - 11:10	S. Apostolov, M. Bivas, N. Ribarska, Intrinsic Transversality and Tangential Transversality, p. 25
11:10 - 11:35	V. Lykina, On Pontryagin Type Maximum Principle for Budget-constrained Infinite Horizon Optimal Control Problems, p. 59
11:35 - 12:00	G. Fusco, Robust Feedback Stabilization by Means of Lyapunov-Like Functions Determined by Lie Brackets, p. 41
	Lunch Break

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Parallel Sessions
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Chairperson	N. Ilieva
09:00 - 09:25	I. Katzarov, N. Ilieva, L. Drenchev, Quantum Effects on 1/2[111] Edge Dislocation Motion in Hydrogen-Charged Fe from Ring-Polymer Molecular Dynamics, p. 53
09:25 - 09:50	P. Petkov, M. Rangelov, N. Iieva, N. Todorova, E. Lilkova, L. Litov, Computational Study of IL-6 Inhibition by Low-Molecular-Weight Heparin, p. 67
09:50 - 10:15	N. Ilieva, P. Petkov, E. Lilkova, L. Litov, Computational Study of Helix Aspersa Mucus Peptides in Complex with a Model Bacterial Membrane, p. 50
	Coffee Break
10:45 - 12:25	*Special Session on "Large-Scale Models: Numerical Methods, Parallel Computations and Applications"*
Chairperson	Z. Zlatev
10:45 - 11:10	A. Penenko, V. Penenko, E. Tsvetova, A. Gochakov, E. Pyanova, V. Konopleva, Sensitivity Operator-Based Approach to Heterogeneous Air Quality Monitoring Data Analysis, p. 66
11:10 - 11:35	V. Ivanov, G. Gadzhev, Behaviour and Scalability of the Hydrostatic and Non-hydrostatic Cores of RegCM Multiscale Simulations on High Performance Computing Platforms, p. 51
11:35 - 12:00	V. Spiridonov, H. Chervenkov, Using the Cauchy Criterion and the Standard Deviation to Evaluate the Sustainability of Climate Simulations, p. 72
12:00 - 12:25	I. Georgieva, G. Gadzhev, Study the Recurrence of the Dominant Pollutants in the Formation of AQI Status over the City of Sofia for the Period 2013-2020, p. 44
	Lunch Break

Thursday, June 10

Parallel Sessions
Lecture Hall C

09:00 - 10:15 *Special Session on "Fractional Diffusion Problems: Numerical Methods, Algorithms and Applications"*

Chairperson P. Vabishchevich

09:00 - 09:25 S. Harizanov, N. Kosturski, I. Lirkov, S. Margenov, Y. Vutov, Reduced Sum Implementation of the BURA Method for Spectral Fractional Diffusion Problems, p. 47

09:25 - 09:50 S. Harizanov, N. Kosturski, I. Lirkov, S. Margenov, Y. Vutov, BURA-based Fractional in Space Diffusion-reaction Approximation Error Analysis, p. 47

09:50 - 10:15 B. Duan, R. Lazarov, J. Pasciak, Robust and Fast Solution of Discrete Equations Involving Fractional Powers of Elliptic Operators, p. 39

Coffee Break

10:45 - 12:00 *Special Session on "Fractional Diffusion Problems: Numerical Methods, Algorithms and Applications"*

Chairperson R. Lazarov

10:45 - 11:10 D. Prodanov, First Order Reaction-diffusion System with Space-fractional Diffusion, p. 68

11:10 - 11:35 T. Danczul, C. Hofreither, On Rational Krylov and Reduced Basis Methods for Fractional Diffusion, p. 38

11:35 - 12:00 P. Vabishchevich, Numerical Solution of Non-Stationary Problems with a Rational Approximation for Fractional Powers of the Operator, p. 76

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Parallel Sessions

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14:25 - 15:40 *Special Session on "Optimal Control of ODEs, PDEs and Applications"*

Chairperson V. Lykina

14:25 - 14:50 D. Ghilli, Mean Field Games Models Arising in Geographical Economic, p. 45

14:50 - 15:15 P. Cannarsa, R. Capuani, P. Cardaliaguet, Mean Field Games with State Constraints, p. 35

15:15 - 15:40 Y. Averboukh, Value Function and Stability Property in the First-order Mean Field Type Differential Games, p. 27

Lecture Hall B

14:00 - 15:40 *Special Session on "HPC and Big Data: Algorithms and Applications"*

Chairperson T. Gurov

14:00 - 14:25 D. Palejev, Numerical Parameter Estimates of Beta-uniform Mixture Models, p. 65

14:25 - 14:50 D. Grigorova, D. Tonchev, D. Palejev, Comparison of Different Methods for Multiple Imputation by Chain Equation, p. 45

14:50 - 15:15 V. Bejanyan, H. Astsatryan, A PGAS-Based Implementation for the Parallel Minimum Spanning Tree Algorithm, p. 29

15:15 - 15:40 A. Iliev, A. Mote, A. Manoharan, Multi-Lingual Emotion Classification using Convolutional Neural Networks, p. 49

Lecture Hall C

14:00 - 15:15 *Special Session on "Fractional Diffusion Problems: Numerical Methods, Algorithms and Applications"*

Chairperson S. Harizanov

14:00 - 14:25 D. Slavchev, S. Margenov, Hierarchical Compression Solver for Parabolic Problems with Space-fractional Diffusion, p. 71

14:25 - 14:50 S. Apostolov, Y. Dimitrov, V. Todorov, Constructions of Second-Order Approximations of the Caputo Derivative, p. 26

14:50 - 15:15 S. Georgiev, L. Vulkov, Parameter Identification Algorithm for a Fractional Dynamics Model of Honeybee Loss, p. 43

Coffee Break

Thursday, June 10

Plenary Session

Chairperson	O. Iliev
16:10 - 16:55	Y. Efendiev, Multiscale Modeling: Modeling Subgrid Effects and Temporal Splitting, p. 39
16:55 - 17:40	X. Hu, Graph Laplacians: Algorithms and Applications, p. 48
17:40 - 18:00	Plenary Closing
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Chairperson	S. Tranev
09:30 - 09:55	V. Traneva, S. Tranev, Intuitionistic Fuzzy Approach for Outsourcing Provider Selection in a Refinery, p. 75
09:55 - 10:20	V. Todorov, I. Dimov, R. Georgieva , S. Apostolov, S. Poryazov, Advanced Stochastic Approaches Based on Optimization of Lattice Sequences for Large-Scale Finance Problems, p. 73
10:20 - 10:45	A. Mucherino, binMeta: a New Java Package for Meta-heuristic Searches, p. 62
10:45 - 11:10	N. Dobrinkova, E. Katsaros, I. Gkotsis, Risk Registry Platform for Optimizations in Cases of CBRN and Critical Infrastructure Attacks, p. 38

Lecture Hall B

09:30 - 11:10	*Special Session on "Large-Scale Models: Numerical Methods, Parallel Computations and Applications"*
Chairperson	K. Georgiev
09:30 - 09:55	T. Ostromsky, V. Todorov, I. Dimov, R. Georgieva, Z. Zlatev, Sensivitity Study of Large-Scale Air Pollution Model Based on Modifications of the Latin Hypercube Sampling Method, p. 64
09:55 - 10:20	V. Todorov, T. Ostromsky, I. Dimov, R. Georgieva, Z. Zlatev, Multidimensional Sensivitity Analysis for AIr Pollution Model Based on Modifications of the Van der Corput Sequence, p. 74
10:20 - 10:45	K. Liolios, G. Skodras, K. Georgiev, I. Georgiev, Effluent Recirculation for Contaminant Removal in Constructed Wetlands under Uncertainty: A Stochastic Numerical Approach Based on Monte Carlo Methodology, p. 58
10:45 - 11:10	A. Alexandrov, R. Andreev, T. Tashev, Large-Scale Simulation Modeling For River Floods Forecasting, p. 23

Part B

Abstracts[2]

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

Monolithic Multigrid for a Reduced-Quadrature Discretization of Poroelasticity

J. Adler

Advanced finite-element discretizations and preconditioners for models of poroelasticity have attracted significant attention in recent years. The equations of poroelasticity offer significant challenges in both areas, due to the potentially strong coupling between unknowns in the system, saddle-point structure, and the need to account for wide ranges of parameter values, including limiting behavior such as incompressible elasticity. The work presented in this talk was motivated by an attempt to develop monolithic multigrid preconditioners for a novel P1-P0-RT-stabilized discretization; we show here why this is a difficult task and, as a result, we modify the discretization through the use of a reduced quadrature approximation, yielding a more "solver-friendly" discretization. Local Fourier analysis is used to optimize parameters in the resulting monolithic multigrid method, allowing a fair comparison between the performance and costs of methods based on Vanka and Braess-Sarazin relaxation. Numerical results are presented to validate the LFA predictions and demonstrate efficiency of the algorithms. Finally, a comparison to existing block-factorization preconditioners is also given.

A Finite-Element Framework for a Mimetic Finite-Difference Discretization of Maxwells Equations

J. Adler, C. Cavanaugh, X. Hu, L. Zikatanov

Maxwells equations are a system of partial differential equations that govern the laws of electromagnetic induction. We study a mimetic finite-difference (MFD) discretization of the equations which preserves important underlying physical properties. We show that, after mass lumping and appropriate scaling, the MFD discretization is equivalent to a structure-preserving finite-element (FE) scheme. This allows for a transparent analysis of the MFD method using the FE framework, and provides an avenue for the construction of efficient and robust linear solvers for the discretized system. In particular, block preconditioners designed for FE formulations can be applied to the MFD system in a straightforward fashion. We present numerical tests which verify the accuracy of the MFD scheme and confirm the robustness of the preconditioners.

Large-Scale Simulation Modeling For River Floods Forecasting

A. Alexandrov, R.Andreev, T.Tashev

One of the aims of the simulation models is to replicate the workings and logic of a real environmental systems by using statistical descriptions of the activities involved.

In the current research is presented a new River Flood Simulation Model (RFSM) using a continuous simulation and machine learning (ML) based flood forecasting.
The proposed approach uses weather generator and by the Large-scale computations, creates a Rainfal-Runoff modell, 1D Channel River Network model, 2D Raster-Based Inertia Model and final Flood Loss model.
Based on the RFSM, is developed a new software algorithm, using real weather statistical data from the Sofia region. The algorithm is able to generate a 3-hours water level forecasting for river Iskar.

New Clustering Techniques of Node Embeddings Based on Metaheuristics

A. Alihodžić, M. Chahin

Node embeddings present a powerful method of embedding graph-structured data into a low dimensional space while preserving local node information. Clustering is a common preprocessing task on unsupervised data utilized to get the best insight into the input dataset. The most prominent clustering algorithm is the K-Means algorithm. In this paper, we formulate clustering as an optimization problem using different objective functions following the idea of searching for the best fit centroid-based cluster exemplars. We also apply several nature-inspired optimization algorithms since the K-Means algorithm is trapped in local optima during its execution. We demonstrate our cluster frameworks' capability on several graph clustering datasets used in node embeddings and node clustering tasks. Performance evaluation and comparison of our frameworks with the K-Means algorithm are demonstrated and discussed in detail. We end this paper with a discussion on the impact of the objective function's choice on the clustering results.

A Comparison of Machine Learning Methods for Forecasting Dow Jones Stock Index

A. Alihodžić, E. Zvornicanin

Stock market forecasting is a challenging and attractive topic for researchers and investors, helping them test their new methods and improve stock returns. Especially in the time of financial crisis, these methods gain popularity. The algorithmic solutions based on machine learning are used widely among investors, starting from amateur ones up to leading hedge funds, improving their investment strategies. This paper made an extensive analysis and comparison of several machine learning algorithms to predict the Dow Jones stock index movement. The input features for the algorithms will be some other financial indices, commodity prices and technical indicators. The algorithms such as decision tree, logistic regression, neural networks, support vector machine, random forest, and AdaBoost have exploited for comparison purposes. The data preprocessing step used

a few normalization and data transformation techniques to investigate their influence on the predictions. In the end, we presented a few ways of tuning hyperparameters by metaheuristics such as genetic algorithm, differential evolution, and immunological algorithm.

A Distributed Epidemiological Model with Vaccination Applied to COVID-19 Pandemic

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

The paper presents a model describing the evolution of an epidemic dis- ease to which vaccination may be applied. The dynamics is modeled by integral equations taking into account the time since infection of the infected individuals, which is especially important for diseases with a relatively long asymptomatic period in which they may be infectious. A key feature is the use of statistical information on the disease status of infected individuals within multiple compartments, while transition rates are not explicitly in- volved. The proposed approach is relevant to Corona Virus Disease 2019 (COVID-19) in the period of scarce vaccination capacity. An optimal con- trol problem is presented, where the aim is to minimize the total number of infected individuals, using as a control policy the allocation of available vaccine to population groups of different level of risk. The talk will focus on the analysis of the model, including optimality conditions, stability analysis and approximations. Numerically obtained optimal vaccination policies will also be presented and discussed.

Intrinsic Transversality and Tangential Transversality

S. Apostolov, M. Bivas, N. Ribarska

Transversality is a classical concept of mathematical analysis and differential topology and it has proven to be useful in variational analysis as well. There are various transversality-type properties reflecting the various needs of the possible applications. The central ones among them are transversality and subtransversality. Recently the notion of intrinsic transversality which is intermediate between subtransversality and transversality has been introduced by Drusvyatskiy, Ioffe and Lewis. All of these notions have been thoroughly studied.

In 2017 A.D. Ioffe posed the question for finding metric characterization of intrinsic transversality as well as characterization of intrinsic transversality in purely tangent terms. This was one of the starting points of our investigation. The other starting point was the notion of tangential transversality which was introduced by Bivas, Krastanov and Ribarska in 2020 while formulating necessary optimality conditions for optimization problems in terms of abstract Lagrange multipliers. Surprisingly it happened that intrinsic transversality and tangential transversality are “almost” equivalent. Thus we

obtained a characterization of intrinsic transversality in tangential terms (having purely metric nature) and proved that it is equivalent in Hilbert spaces to a characterization of intrinsic transversality obtained by Thao, Bui, Cuong and Verhaegen (2020).
Establishing the exact relationship between intrinsic transversality and tangential transversality helped us to obtain characterizations in tangential terms of both transversality and subtransversality close in nature to tangential transversality. There have been known primal sufficient conditions and primal necessary conditions for transversality and subtransversality, but no primal characterizations.

Constructions of Second-Order Approximations of the Caputo Derivative

S. Apostolov, Y. Dimitrov, V. Todorov

In previous papers we derive approximations of the second derivative, whose the generating functions are transformations of the exponential and the logarithmic functions.

$$\frac{1}{h^2}\sum_{k=0}^{n} w_{i,k} f(x-kh) = f''(x) + O(h), \tag{1}$$

$$w_{1,0} = 2A\left(1 - A + Ae^{-1/A}\right),\ w_{1,1} = -2A\left(1 - e^{-1/A}\right),\ w_{1,k} = \frac{2e^{-1/A}}{k!A^{k-2}},$$
$$w_{2,0} = \frac{2(B - \ln(B+1))}{B^2}, \qquad w_{2,1} = -\frac{2}{B+1}, \qquad w_{2,k} = \frac{2B^{k-2}}{k(B+1)^k},$$

where $h = (x_0 - x)/n$. Approximations (1) hold for all functions $f \in C^2[x_0, x]$ when the weights $w_{i,n-1}$ and $w_{i,n}$ satisfy

$$w_{i,n-1} = \sum_{k=0}^{n-2}(k-n)w_{i,k}, \qquad w_{i,n} = \sum_{k=0}^{n-2}(n-k-1)w_{i,k}, \qquad (i = 1, 2).$$

By substituting the second derivative in the expansion formula of the L1 approximation with (1) we obtain second-order approximations of the Caputo derivative with a lower limit x_0

$$\frac{1}{h^\alpha}\sum_{k=0}^{n} w_{i,k}^{(\alpha)} f(x-kh) = f^{(\alpha)}(x) + O\left(h^2\right). \tag{2}$$

In the present paper we prove that for every $\alpha \in (0, 1)$ there exist values of A and B such that the weights of approximations (2) satisfy

$$w_{i,0}^{(\alpha)} > 0, \quad w_{i,1}^{(\alpha)} < w_{i,2}^{(\alpha)} < \cdots < w_{i,n-2}^{(\alpha)} < 0, \tag{3}$$

and we derive estimates for the parameters A and B with respect to the order α of fractional differentiation. Applications of approximations (2) for numerical solution of fractional differential equations are given in the paper. Properties (3) of the weights are used in the convergence analysis of the numerical solutions.

On the Use of Low-Discrepancy Sequences in the Training of Neural Networks

E. Atanassov, D. Georgiev, T. Gurov

The quasi-Monte Carlo methods use specially designed deterministic sequences with improved uniformity properties compared with random numbers, in order to achieve higher rates of convergence. Usually certain measures like the discrepancy are used in order to quantify these uniformity properties. The usefulness of certain families of sequences with low discrepancy, like the Sobol and Halton sequences, has been established in problems with high practical value as in Mathematical Finance. Multiple studies have been done about applying these sequences also in the domains of optimisation and machine learning. Currently many types of neural networks are used extensively to achieve break-through results in Machine Learning and AI. The process of training these networks requires substantial computational resources, usually provided by using powerful GPUs or specially designed hardware. In this work we study different approaches to employ efficiently low-discrepancy sequences at various places in the training process where their uniformity properties can speed-up or improve the training process. We demonstrate the advantage of using Sobol low-discrepancy sequences in benchmark problems and we discuss various practical issues that arise in order to achieve acceptable performance in real-life problems.

Value Function and Stability Property in the First-Order Mean Field Type Differential Games

Y. Averboukh

We study the collective behavior of infinitely many agents governed by two players with opposite purposes under assumption of the mean field interaction between the agents. The whole system is considered as a control system in the space of probability measures endowed with the Wasserstein (Kantorovich) metric. We assume that the dynamics of each agent is given by the ODE

$$\frac{d}{dt}x\left(t\right)=f\left(t,x\left(t\right),m\left(t\right),u\left(t\right),v\left(t\right)\right).$$

Here, $t\in[0,T]$ denotes a time, $x\left(t\right)$ is a state of the agent, $m\left(t\right)$ is the distribution of all agents at time t; $u\left(t\right)\in U$ (respectively, $v\left(t\right)\in V$) is the control of the first (respectively, second) player acting on the agent; U (respectively, V) is the control space for the first (respectively, second) player. For simplicity it is assume that the phase space for each agent is d-dimensional flat torus.
We assume that the first player tries to minimize the terminal payoff

$$g\left(m\left(t\right)\right)$$

The purpose of the second player is opposite. The main results of the talks are as follows. First, we introduce so called u- and v-stability properties and show that, given u-stable (resp. v-stable) function, one can construct a suboptimal strategy of the first (resp. second) player. Thus, u-stable (resp. v-stable) functions are upper (resp. lower) bounds of the value function. Then, we prove the existence of the value function showing that there exists a function that is u- and v-stable simultaneously. Finally, we present the infinitesimal forms of the stability conditions using analogs of directional derivatives.

An Exact Schur Complement Method for Time-harmonic Optimal Control Problems

O. Axelsson, D. Lukáš, M. Neytcheva

By use of Fourier time series expansions in an angular frequency variable, time-harmonic optimal control problems constrained by a linear differential equation decouples for the different frequencies. Hence, for the analysis of a solution method one can consider the frequency as a parameter. There are three variables to be determined, the state solution, the control variable and the adjoint variable.
The first order optimality conditions lead to a three-by-three block matrix system where the adjoint optimality variable can be eliminated. For the so arising two-by-two block system, in this paper we study a factorization method involving an exact Schur complement method.
We illustrate the performance of the proposed preconditioning method in its inexact version on the discrete optimal control problem with a constraint, given by the time-harmonic eddy current problem in a three dimensional space domain. The numerical experiments show that the convergence is independent of the discretization parameter as well as of the regularization parameter and the angular frequency.

Optimal Knock-Out Tournaments: Definition and Computation

A. Bădică, C. Bădică, I. Buligiu, L. I. Ciora, D. Logofătu

In this paper we introduce our own formal definition of competitions that have the shape of hierarchical single-elimination tournaments, also known as *knockout tournaments*. We introduce methods to quantitatively evaluate the attractiveness / competitiveness of a given tournament. We consider that a tournament is more attractive / competitive if topmost players will have the chance to meet in higher stages of the tournament, thus increasing the stake of their matches.
In knockout tournaments, the result of each match is always a win of one of the two players, i.e. draws are not possible. A knockout tournament with n stages is structured as a complete binary tree with 2^n leaves. Each leaf represents one player or team that is enrolled in the tournament, while each internal node represents a match of the tournament.

We provide an exact formula for counting the total number of n-stage knockout tournaments, showing that the number of tournaments grows very large with the number of players $N = 2^n$.
We define the set of possible matches at each stage. Based on this observation we show that for each two players i and j and a given tournament there is a unique stage of the tournament where the players can meet. We assign a quota to each player such that higher ranked players have a larger quota. This allows us to define a cost function of a tournament based on players' quota that assigns a higher cost to those tournaments where highly ranked players will tend to meet in the higher stages, thus making the tournament more attractive and competitive.
The cost of a tournament for a given set of players can be defined recursively based on the cost of two half-sized tournaments defined by a 2-partition of the set of players. This observation allows us to define a dynamic programming algorithm for computing the optimal knockout tournament given by a set of players and their ranks. The state space of this algorithm is defined by a subset of the power-set of the set of players that has an exponential size in the number of players. It follows that this algorithm consumes exponential time and memory in the number N of players enrolled in the tournament.

On the Consistency Order of Runge–Kutta Methods Combined with Active Richardson Extrapolation

T. Bayleyegn, I. Faragó, Á. Havasi

Passive and active Richardson extrapolations are robust devices to increase the rate of convergence of time integration methods. While the order of convergence is shown to increase by one under rather natural smoothness conditions if the passive Richardson extrapolation is used, for the active Richarson extrapolation the increase of the order has not been generally proven. It is known that the Lipschitz property of the right-hand side function of the differential equation to be solved yields convergence of order p if the method is consistent in order p. In this paper it is shown that the active Richardson extrapolation increases the order of consistency by one when the underlying method is any RungeKutta method of order $p = 1; 2$ or 3.

A PGAS-Based Implementation for the Parallel Minimum Spanning Tree Algorithm

V. Bejanyan, H. Astsatryan

The minimum spanning tree is a critical problem for many applications in network analysis, communication network design, and computer science. The parallel implementation of minimum spanning tree algorithms increases the simulation performance of large graph problems using high-performance computational resources. The minimum spanning tree

algorithms generally use traditional parallel programming models for distributed and shared memory systems, like Massage Passing Interface or OpenMP. Furthermore, the partitioned global address space model offers new capabilities in the form of asynchronous computations on distributed shared memory, positively affecting the performance and scalability of the algorithms. The paper aims to present a new minimum spanning tree algorithm implemented in a partitioned global address space model. The experiments with diverse parameters have been conducted to study the efficiency of the asynchronous implementation of the algorithm.

A New Error Estimate for a Primal-Dual Crank Nicolson Mixed Finite Element using Lowest Degree Raviart Thomas Spaces for Parabolic Equations

F. Benkhaldoun, A. Bradji

We consider the heat equation

$$u_t(\mathbf{x},t) - \Delta u(\mathbf{x},t) = f(\mathbf{x},t), \qquad (\mathbf{x},t) \in \Omega \times (0,T),$$

with homogeneous Dirichlet boundary conditions where Ω is an open polygonal bound-ed subset in $\mathbb{R}^d$, f is a given function defined on $\Omega \times (0,T)$, and $T > 0$. We consider a fully discrete scheme based on the use of Primal-Dual Lowest Order Raviart Thomas Mixed method combiined with a Crank-Nicolson method, that is we perform finite element approximation using Lowest Degree Raviart Thomas spaces in space and the Crank-Nicolson finite difference method in time, of the equivalent system: Find $(p,u) : (0,T) \longrightarrow H_{\text{div}}(\Omega) \times L^2(\Omega)$ such that

$$(u_t, \varphi)_{L^2(\Omega)} + (\text{div}p, \varphi)_{L^2(\Omega)} = (\varphi, f)_{L^2(\Omega)}, \qquad \forall \varphi \in L^2(\Omega) \tag{1}$$

and

$$(p, \psi)_{L^2(\Omega)} = (u, \text{div}\psi)_{L^2(\Omega)} \qquad \forall \psi \in H_{\text{div}}(\Omega). \tag{2}$$

We prove new convergence results with convergence rates towards $(-\nabla u(t), u(t))$ in the discrete norms of $L^2(H_{\text{div}}(\Omega)) \times H^1(L^2(\Omega))$, under assumption that the solution is smooth. The order in time is two and is one in space. These results are obtained thanks to some new well developed discrete a priori estimates. The convergence results obtained in this work improve the known existing ones for PDMFEM (Primal-Dual Mixed Finite Element Method) for Parabolic equations which state the convergence towards only $(-\nabla u(t), u(t))$ in the discrete norms of $L^\infty(L^2(\Omega)^d) \times L^\infty(L^2(\Omega))$. It is useful to mention that, there are already similar results in the literature of PDMFEM for **Elliptic Equations** in the sense that the convergence of MFEM is proved towards $(-\nabla u, u)$ in the discrete norms of $H_{\text{div}}(\Omega) \times L^2(\Omega)$.
In addition to this, many of authors applies the so-called Primal Mixed Finite Element, i.e. a mixed formulation based on the use of the spaces $L^2(\Omega)^d$ and $H^1(\Omega)$ (instead of the spaces $H_{\text{div}}(\Omega)$ and $L^2(\Omega)$), when dealing with Crank-Nicolson finite difference method as discretization in time

A Finite Volume Scheme for a Wave Equation with Several Time Independent Delays

F. Benkhaldoun, A. Bradji, T. Ghoudi

We establish a finite volume scheme for a second order hyperbolic equation with Several Time Independent Delays in any space dimension. This model is considered in some previous works where some exponential stability estimates or some oscillations results are proved. The scheme uses, as space discretization, SUSHI (Scheme using Stabilization and Hybrid Interfaces). We first prove the existence and uniqueness of the discrete solution. We subsequently, develop a new discrete *a priori estimate*. Thanks to this *a priori estimate*, we prove error estimates in several discrete seminorms.

A Deep Learning Approach to Operator Inference

P. Benner, P. Goyal, I. P. Duff

Mathematical modeling of dynamical processes is essential to understand their transient and long-term behavior, and to perform engineering tasks such as control and design optimization. With the increasing of accessibility of data, learning models directly from data recently has drawn a lot of attention. Moreover, it is desirable to construct compact low-dimensional models describing complex non-linear dynamics, allowing to perform simulations and optimization studies on modest computer hardware. To that aim, the construction of low-order models is well reflected in the recent successes of data-driven approaches such as Dynamic Mode Decomposition (DMD) and Operator Inference (OpInf). Physical interpretability of models learned from data relies on the incorporation of known physical constraints (e.g., mass conversation, energy conversation) in the learning models. In light of this, we discuss a tailored OpInf approach for learning low-order models for high fidelity non-linear systems, which leverages the additional knowledge about the physical process to be modeled. In particular, we suggest to combine OpInf with certain deep neural network approaches to infer the unknown nonlinear dynamics of the system. This requires to encode the physical constraints like conservation laws in into the network architecture. We suggest OpInf network architectures that achieve these tasks for several often encountered engineering problems like flow control. We will show the performance of the proposed method to learning low-dimensional models using simulated data and compare it with projection-based (intrusive) methods that require (and benefit from) the availability of a known high-fidelity model as well as to other data-driven approaches.

Robust Preconditioners for Perturbed Saddle-Point Problems and Conservative Discretizations of Biot'S Equations Utilizing Total Pressure

W. M. Boon, M. Kuchta, K.-A. Mardal, R. Ruiz-Baier

We develop robust solvers for a class of perturbed saddle-point problems arising in the study of a second-order elliptic equation in mixed form (in terms of flux and potential), and of the four-field formulation of Biot's consolidation problem for linear poroelasticity (using displacement, filtration flux, total pressure and fluid pressure). The stability of the continuous variational mixed problems, which hinges upon using adequately weighted spaces, is addressed in detail; and the efficacy of the proposed preconditioners, as well as their robustness with respect to relevant material properties, is demonstrated through several numerical experiments.

Hybrid Mimetic Finite-Difference and Virtual Element Formulation for Coupled Poromechanics

A. Borio, F. Hamon, N. Castelletto, J. A. White, R. R. Settgast

We present a fully implicit hybrid mimetic finite-difference and virtual element formulation for coupled poromechanics on unstructured meshes. The proposed scheme is convergent on complex meshes containing highly distorted cells with arbitrary shapes. A scalable iterative linear solution strategy is obtained using a block-triangular preconditioner designed specifically for the saddle-point systems arising from the discretization. We demonstrate the validity of our fully coupled approach using poromechanical problems in two and three dimensions, particularly showing the advantages of using polytopal meshes.

An Accelerated Staggered Scheme For Phase-field Models Of Hydraulic Fracture In Poroelastic Media

J. W. Both, J. M. Nordbotten, F. A. Radu, J. M. Sargado, E. Storvik

Fluid flow in fractured, deformable porous media is of high relevance in applications ranging from geological to industrial applications as, e.g., geothermal energy. In particular, hydraulic fracturing takes a major role in the stimulation and operation of enhanced geothermal systems.
Flow in deformable porous media is commonly described by the quasi-static Biot equations for poroelastic media. Furthermore, a popular approach for modeling brittle fracture is to use phase-field models. Instead of resolving fractures as sharp entities, they are

smeared out and represented by an additional variable, characterized by an additional model equation. In this work, we consider a fully coupled model, coupling fluid flow, deformation, and fracturing via phase-fields.
For both, poroelasticity models as well as phase-field models, staggered solution schemes are widely used. In particular, for coupled poroelasticity models, they serve as basis for efficient and flexible solver technology, whereas for phase-field models staggered schemes are often employed due to their increased robustness compared to monolithic schemes. However, for the latter staggered schemes may become quite slow in situations of brutal fracturing. In a recent work, we have proposed acceleration strategies combining overrelaxation and Anderson acceleration to mitigate this issue.
In this work, we extend previous efforts and propose a staggered scheme for the coupled model for hydraulic fracture in poroelastic media and enhance its convergence by a similar acceleration strategy. The efficiency and robustness of the approach will be analyzed based on numerical examples.

Bilinear Control of Parabolic Evolution Equations

F. A. Boussouira, P. Cannarsa, C. Urbani

Despite the importance of control systems governed by bilinear controls for the description of phenomena that could not be modeled by additive controls, such as for instance the vibration of a beam composed by *smart materials*, or the process of increasing the speed of a chemical reaction by adding *catalysts*, the action of multiplicative controls is generally not so widely studied as it happens for boundary and locally distributed controls. The main reasons of this fact might be found in the intrinsic nonlinear nature of such problems and furthermore, for controls that are scalar functions of time, in an ineluctable obstruction for proving results of exact controllability which is contained in the celebrated work of Ball, Marsden and Slemrod pubblished in 1982. Nevertheless, one could study *controllability to a trajectory* which is a similar problem to the classical *controllability along a trajectory*.
In this talk I will present results of stabilization and controllability for evolution equations of parabolic type via bilinear control to some particular targets called *eigensolutions*. Then, I will apply our abstract results to the bilinear heat equation with different boundary conditions and to a degenerate parabolic equation.

Bootstrap AMG

J. Brannick

This talk focuses on developing a generalized bootstrap algebraic multigrid algorithm for solving discretized partial differential equations. As a motivation of the proposed generalization, we consider an optimal form of classical algebraic multigrid interpolation that has as columns eigenvectors with small eigenvalues of the generalized eigen-problem

involving the system matrix and its symmetrized smoother. We use this optimal form of interpo- lation to design an algorithm for choosing and analyzing the suitability of the coarse grid. In addition, it provides insights into the design of the bootstrap algebraic multigrid setup algorithm that we propose, which uses as a main tool a multilevel eigensolver to compute approximations to these generalized eigenvectors. A notable feature of the approach is that it allows for general block smoothers and, as such, is well suited for systems of partial differential equations.

Interface Preconditioners for Multiphysics Problems

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

Our work concerns preconditioners for multiphysics problems with a special interest in interfacial coupling. This coupling is usually imposed by the Lagrange multiplier that enforces constraints on the interface, while in domains at each side of the interface different physical laws can govern. Typical examples can be found in geo- and biophysics, such as coupling of free flow and porous media flow or coupling of physical laws across dimensions. The preconditioners for the interface problems are derived on weighted fractional Sobolev spaces, resulting to be represented as a sum of fractional Laplacian operators that can include both negative and positive fractionalities. For that, we implement two approaches to handling the fractional operators numerically.
We first present the factorization-based approach to handling the sum of fractionalities, which results in a multiplicative solver. It consists of an inner elliptic operator which solved using the standard algebraic multigrid method, while special smoothers are implemented for the outer fractional operators. Alternatively, our second approach uses the rational approximation method as an additive solver that represents the fractional power function as a sum of rational functions.
We show scalability, robustness and efficiency of our methods on several numerical examples, including Darcy-Stokes and mixed-dimensional problems.

Modeling and Optimal Control of an Octopus-like Soft Manipulator

S. Cacace, A.C. Lai, P. Loreti

We present a control model for an octopus-like soft manipulator, based on the dynamics of an inextensible string representing the symmetry axis of the device, subject to curvature constraints and curvature controls. The model results in a system of fourth-order evolutive nonlinear controlled PDEs, generalizing the classical Euler-Bernoulli beam equation. We investigate some reachability and grasping problems in the framework of optimal control theory of PDEs, both in stationary and dynamic settings, including cases modelling hyper-redundant manipulators, mechanical breakdowns of the soft actuators, and also problems in constrained environments.

Finally, we discretize the system via finite differences, and we numerically solve some optimal control problems employing suitable augmented Lagrangian and adjoint-based gradient descent methods.

Approximation of Hamilton-Jacobi-Bellman Equations with Neumann Boundary Conditions

E. Calzola, E. Carlini, X. Dupuis, F. J. Silva

We propose a first order explicit semi-Lagrangian method to approximate the solution of the following stochastic control problem on a bounded domain. Let $\mathcal{O} \subseteq \mathbb{R}^d$ (with $d = 1, 2, 3$) be an open bounded set, we consider the problem

$$\begin{cases} -\partial_t u(t,x) + \max\limits_{a \in A} H\left(t, x, Du, D^2u, a\right) = 0 \quad \text{for } (0,T) \times \mathcal{O}, \\ \max\limits_{b \in B} \left\{ \langle \gamma(x,b), Du \rangle - g(t,x,b) \right\} = 0 \quad \text{for } (t,x) \in (0,T) \times \partial\mathcal{O}, \\ u(T,x) = u_T(x) \quad \text{for } x \in \overline{\mathcal{O}}, \end{cases} \tag{1}$$

where $T > 0$, A and B are compact sets, $\langle n(x), \gamma(x,b) \rangle > \nu > 0$ for all $x \in \partial\mathcal{O}$, with n outward-pointing normal to $\mathcal{O}$, and

$$H(t,x,p,M,a) = -\frac{1}{2}\mathrm{Tr}\left(\sigma(t,x,a)\sigma(t,x,a)^\top M\right) - \langle \mu(t,x,a), p \rangle - f(t,x,a),$$

for some μ, σ and f such that a comparison principle holds. σ is a positive semidefinite matrix, possibly degenerate. Firstly, we discretize the solution of the stochastic SDE for the characteristic curves using the stochastic Euler method, then we reconstruct the numerical solution at the feet of the characteristics using standard interpolation techniques on unstructured spatial grids. The main novelty of our approach is in the treatment of non-linear Neumann-type boundary conditions: each time one of the characteristics falls outside of the spatial domain, it is reflected inside along a direction depending both on the position of the characteristic itself and on the vector field γ. Finally, the numerical solution interpolated in the reflected point is corrected with a term depending on the boundary condition g. We have proved consistency, stability and convergence of this scheme. We underline that those results hold under an inverse parabolic CFL condition, which allows for large time steps. In the end, we concluded our work with some numerical simulations, both in $\mathbb{R}$ and in $\mathbb{R}^2$.

Mean Field Games with State Constraints

P. Cannarsa, R. Capuani, P. Cardaliaguet

This talk will address deterministic mean field games for which agents are restricted in a closed domain with smooth boundary. In this case, the existence and uniqueness of Nash

equilibria cannot be deduced as for unrestricted state space because, for a large set of initial conditions, the uniqueness of solutions to the minimization problem which is solved by each agent is no longer guranteed. Therefore we attack the problem by considering a relaxed version of it, for which the existence of equilibria can be proved by set-valued fixed point arguments. Then, we give a uniqueness result for such equilibria under a classical monotonicity assumption. Finally, by analyzing the regularity and sensitivity with respect to space variables of the relaxed solution, we will show that it satisfies the MFG system in suitable point-wise sense.

Evolution Equations in Wasserstein Spaces Ruled by Probability Vector Fields

G. Cavagnari

We present recent results framing into the theory of *Measure Differential Equations* introduced by B. Piccoli (Rutgers University-Camden). The dynamics is set in the Wasserstein space of probability measures. Moreover, also the action of the vector filed itself is given by a probability measure living on the tangent bundle. To deal with evolutions in the Wasserstein space, tools of Optimal Transport are essential.
In this work, we build a stronger notion of solution for which we are able to get existence, uniqueness and stability results. This is based on ideas coming from the theory of evolution equations driven by *dissipative operators* on Hilbert spaces, according to which we give a notion of solution in terms of a so called *Evolution Variational Inequality*. Finally, we are able to compare this stronger notion with the original one, showing that our construction "selects" one of the (not unique) solutions in the sense of Piccoli.
This is a joint work with G. Savaré (Bocconi University) and G. E. Sodini (TUM-IAS).

State Constrained Control Problems and Second Order Inward Pointing Conditions

G. Colombo, N. T. Khalil, F. Rampazzo

We investigate a class of state-constrained controlled dynamical systems where the classical first order inward pointing condition, also known as Soner's condition, is violated. In these circumstances, given an initial point, the construction of trajectories belonging to the interior of the state constraint is not possible in general. The first feature of this paper is to prove that under a *higher order inward pointing condition*, together with some other assumptions involving the vector fields and the constraint, a novel construction guarantees the existence of such interior trajectories. Subsequently, using the above construction we derive a *neighboring feasible trajectories* result which allows to approximate any reference trajectory (possibly violating the state constraint) by a feasible one.

Moreover, our result encompasses a *non-linear* estimate of the distance of a given reference trajectory from the set of feasible state trajectories, while the estimate is linear (or super-linear) in previous works. Some examples are presented to support the analysis. As an application, we establish the continuity of the value function of general optimal control problems up to the boundary of the constraint.

Model Predictive Control for Affine Problems

A. D. Corella

The talk will discuss an implementation of a Model Predictive Control (MPC) algorithm to affine optimal control problems containing a uncertain time-dependent parameter, for which only a predicted (reference) information is known. More precisely, we consider finite-horizon continuous time optimal control problems which are affine with respect to the control variable. After discretizing the problem, we employ an MPC approach by first solving the reference problem over the entire remaining time horizon and then applying the first element of the optimal discrete-time control sequence, as a constant in time control function, to the continuous system over the sampling interval. Then the state at the end of the sampling interval is estimated with certain error, and the process is repeated at each step over the remaining horizon. As a result, we obtain a piece-wise constant function representing the MPC-generated control signal. We obtain estimations for the difference of this MPC-generated control and the optimal control for reference problem. The talk is based on a joint work with Vladimir M. Veliov.

Scalable Preconditioners for Computational Science at Extreme Scale

P. D'Ambra, F. Durastante, S. Filippone

The challenge of exascale requires a rethinking of algorithms and software for efficient exploitation of heterogeneous massively parallel supercomputers. In this talk we present some activities aimed to develop highly scalable and robust sparse linear solvers for solving scientific and engineering applications with a huge number of degrees of freedom. We discuss algorithmic advances and implementation aspects for designing Algebraic MultiGrid (AMG) preconditioners to be used in conjunction with the Krylov-subspace projection methods and their use in some applications arising from the EoCoE-II project. Results obtained with the PSBLAS and AMG4PSBLAS libraries, on some of the most powerful European supercomputers, for solving systems of dimension up to $O(10^{10})$ arising from isotropic and anisotropic scalar elliptic PDEs, will be presented.

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On Rational Krylov and Reduced Basis Methods for Fractional Diffusion

T. Danczul, C. Hofreither

We establish an equivalence between two classes of methods for solving fractional diffusion problems, namely, Reduced Basis Methods (RBM) and Rational Krylov Methods (RKM). In particular, we demonstrate that several recently proposed RBMs for fractional diffusion, namely those by [Danczul, Schöberl], by [Bonito, Guignard, Zhang], and by [Dinh, Antil, Chen, Cherkaev, Narayan], can be interpreted as RKMs. This changed point of view allows us to give convergence proofs for some methods that did not have such a proof previously.
We also propose a new RKM for fractional diffusion problems with poles chosen using the best rational approximation of the function x^{-s} in the spectral interval of the spatial discretization matrix. The poles are computed using the BRASIL algorithm for best rational approximation recently proposed by the second author. We prove convergence rates for this RKM and demonstrate numerically that it is competitive with or superior to many methods from the reduced basis, rational Krylov, and direct rational approximation classes.

Isogeometric Analysis for Poroelasticity

Á. P. de la Riva, F. J. Gaspar, C. Rodrigo

The theory of poroelasticity models fluid flow within a deformable porous media and it has been extensively studied in the literature due to its wide range of applications in different areas such as geosciences and biomedicine for example. The numerical simulation of this type of problems requires both an appropriate discretization scheme and the design of an efficient solution method for the large systems of equations that arise after discretization. Here, we consider a discretization of the problem based on isogeometric analysis. In particular, Taylor Hood type elements will be considered. The main focus of this work, however, is to propose an efficient solver that takes advantage of the decoupling of the flow and the mechanics within a fixed-stress split scheme. The main advantage of the proposed method will be its robustness with respect to the spline degrees considered within the isogeometric discretization.

Risk Registry Platform for Optimizations in Cases of CBRN and Critical Infrastructure Attacks

N. Dobrinkova, E. Katsaros, I. Gkotsis

Nowadays the world faces a wide range of complex challenges and threats to its security. The origination of modern threats, among others takes into consideration the proliferation

of weapons of mass destruction (WMD) and their delivery systems. Rapid advances in science and technology, have proven to be misused by terrorist groups who develop the necessary knowledge and capacity to turn them in Chemical-biological-radiological and nuclear threats against the civil population. Adequate response and cross-sectoral cooperation in case of emergency situation is the base for low number of casualties and fast localization of the threat source. Risk Registry tools used to optimize the CBRN and critical infrastructure attacks are important crisis management capacity which need to be further developed using the nowadays information and communication technologies (ICT). Identifying and formulating registry algorithms containing documented cases of realized threats in these thematic areas including data on the technological side of attacks is very important for tactical planning. In our paper we will describe a Risk Registry platform and its and implementation for optimization purposes.

Robust and Fast Solution of Discrete Equations Involving Fractional Powers of Elliptic Operators

B. Duan, R. Lazarov, J. Pasciak

We develop and study an algorithm for approximately solving the linear algebraic system $\mathcal{A}_h^\alpha u_h = f_h$, $0 < \alpha < 1$, where the finite dimensional operator $\mathcal{A}_h$ is obtained from an approximation scheme for a second order elliptic problems, e.g., finite element/difference scheme or spectral or spectral element methods, as long as the corresponding mass and stiffness matrices are sparse and the resulting linear system can be solved efficiently. Due to P. Vabishchevich, the solution of this problem is related to the solution of an initial value problem of a certain pseudo-parabolic equation, in fact this is a system of dimension d, with d being the dimension of $\mathcal{A}_h$. We propose a stable and exponentially convergent time stepping scheme based on Padé approximation. The rigorous analysis shows that the asymptotic cost of the proposed scheme is solving $\mathcal{O}(\log_2 d)$ sparse systems. The numerical tests demonstrate the efficiency of the proposed scheme and confirm the theoretical analysis findings.

Multiscale Modeling: Modeling Subgrid Effects and Temporal Splitting

Y. Efendiev

In this talk, we will start with some main concepts in multiscale modeling including numerical homogenization and multiscale finite element methods. Our goal is to model processes in multiscale media without scale separation and with high contrast. We assume that the coarse grid doesnt resolve the scales and the contrast. To deal with these problems, I will introduce multiscale methods that use multicontinua approaches. These approaches use additional macroscopic variables. I will discuss the convergence of these

approaches and show that these methods converge independent of the contrast. The multicontinua approaches can benefit from machine learning techniques, which I will discuss. I will also consider how multiscale methods can be used for temporal splitting. High contrast brings stiffness to the system, which requires small time steps. We will introduce partial explicit methods that construct time discretizations with the time stepping that is independent of the contrast. Numerical results will be shown to back up our theories.

Scalable Solvers for Hybridized Coupled Poromechanics

M. Ferronato, M. Frigo, N. Castelletto, J. A. White

A stabilized mixed hybrid finite element formulation for three-field (displacement-pressure-velocity) coupled poromechanics is considered. When using low-order elements, namely piecewise linear for displacements, piecewise constant for pressures and lowest-order Raviart-Thomas for velocities, the stabilization strategy, based on a macro-element approach, is required to eliminate the spurious pressure modes appearing in undrained/incompressible conditions.
The iterative solution of the resulting block system is addressed by developing a class of block triangular preconditioners based on a Schur-complement approximation strategy. Theoretical results are first provided, proving: (i) the boundedness of the eigenspectrum of the preconditioned matrix, and (ii) the regularity of the Schur complement for any time-step size and material properties. Computational efficiency and scalability are then tested in challenging real-world applications. The use of a hybridized discretization approach allows for a superior performance with respect to standard mixed methods with heterogeneous and anisotropic materials. Finally, a nearly optimal scalability, in both the weak and strong sense, is verified in massively parallel applications.

Influence of the ACO Evaporation Parameter for Unstructured Workforce Planning Poblem

S. Fidanova, O. Roeva

Optimization of the production process is important for every factory or organization. The better organization can be done by optimization of the workforce planing. The main goal is decreasing the assignment cost of the workers with the help of which, the work will be done. The problem is NP-hard, therefore it can be solved with algorithms coming from artificial intelligence. The problem is to select employers and to assign them to the jobs to be performed. The constraints of this problem are very strong and for the algorithms is difficult to find feasible solutions espesially when the problem is unstructured. We apply Ant Colony Optimization Algorithm to solve the problem. We investigate the algorithm performance according evaporation parameter. The aim is to find the best parameter setting.

Deep Neural Networks and Adaptive Quadrature for Solving Variational Problems

D. Fokina, O. Iliev, I. Oseledets

The great success of deep neural networks (DNNs) in such areas as image processing, natural language processing has motivated also their usage in many other areas. It has been shown that in particular cases they are provide very good approximation to different classes of functions. The aim of this work is to explore the usage of deep learning methods for approximation of functions, which are solutions of boundary value problems for particular differential equations. More specific, the class of methods known as Physics Informed Neural Network will be explored. Components of the DNN algorithms, such as the definition of loss function, the choice of activation function, the choice of the minimization method, the DNN architecture, will be discussed while presenting results from the computational experiments.

Robust Feedback Stabilization by Means of Lyapunov-Like Functions Determined by Lie Brackets

G. Fusco

We use Lie brackets of unbounded vector fields in order to consider a dissipative relation that generalizes the differential inequality which defines classic control Lyapunov functions. Under minimal regularity assumptions, we employ locally semiconcave solutions of this extended relation, called *degree-k control Lyapunov functions*, in order to design *degree-k Lyapunov feedbacks*, that is, particular discontinuous feedback laws that stabilize the underlying system to a given closed target with compact boundary, in the sample and hold sense. We also prove that this feedback construction is robust when small measurement errors and external disturbances occur.

Nondegenerate Abnormality, Controllability, and Gap Phenomena in Optimal Control with State Constraints

G. Fusco, M. Motta

In optimal control theory, *infimum gap* means that there is a gap between the infimum values of a given minimum problem and an extended problem, obtained by enlarging the set of original solutions and controls. The gap phenomenon is somewhat "dual" to the problem of the *controllability* of the original control system to an extended solution. In this paper we present sufficient conditions for the absence of an infimum gap and for controllability for a wide class of optimal control problems subject to endpoint and state

constraints. These conditions are based on a nondegenerate version of the nonsmooth constrained maximum principle, expressed in terms of subdifferentials. In particular, under some new constraint qualification conditions, we prove that: (i) if an extended minimizer is a *nondegenerate normal* extremal, then there is no gap; (ii) given an extended solution verifying the constraints, either it is a *nondegenerate abnormal* extremal, or the original system is controllable to it. An application to the impulsive extension of a free end-time, non-convex optimization problem with control-polynomial dynamics illustrates the results.

A Full Order, Reduced Order and Machine Learning Model Pipeline for Efficient Prediction of Reactive Flows

P. Gavrilenko, B. Haasdonk, O. Iliev, M. Ohlberger, F. Schindler, P. Toktaliev, T. Wenzel, M. Youssef

Reactive transport in porous media in connection with catalytic reactions is the basis for many industrial processes and systems, such as fuel cells, photovoltaic cells or catalytic filters. The modeling and simulation of the processes can help in optimizing the design of catalytic components, but is currently limited by the fact that such simulations lead to large amounts of data, are time-consuming and depend on a large number of parameters. The development of solution approaches for the prediction of the chemical conversion rate using modern data-based methods is essential in order to achieve fast, reliable predictive models. Various method classes are required for this. In addition to the experimental data, fully resolved simulations are necessary. However, these are too expensive to generate a large set of training data. Therefore, model order reduction is crucial for acceleration as it can produce large amounts of training data.
In this talk we consider projection based model order reduction of linear reactive flow with different flow regimes, i.e. for the advection-diffusion-reaction problem for a concentration c

$$\partial_t c - \Delta c + P_e \nabla \cdot (uc) + D_a c = 0,$$

with appropriate initial and boundary conditions, for varying flow fields u as well as Damkhler and Péclet numbers $D_a, P_e > 0$. While the approximation by discretization schemes and model order reduction (by e.g. Reduced Basis methods) of such problems is well understood, the characteristics of the underlying flow, and thus the solution manifold, may differ significantly if Damkhler and Péclet numbers change by several orders of magnitude. We thus consider practical implications of strongly varying Damkhler and Péclet numbers on stable and accurate reduced order models for such problems, which are then used for generating training data within the collaborative BMBF-funded project on *Machine Learning and Model Order Reduction to Predict the Efficiency of Catalytic Filters (ML-MORE).*

Tensor Networks of Sparse Non-Negative Tensors

P. G. Georgiev

We develop tensor decomposition methods for sparse non-negative tensors, which can be considered as analogs of tensor train and hierarchical decompositions for general tensors. Combined, these decompositions can be considered as tensor networks for non-negative tensors. The key technique uses a fast non-negative matrix factorization algorithm exploiting a mild sparseness of the data. Some applications are given to signal separation problems.

Parameter Identification Algorithm for a Fractional Dynamics Model of Honeybee Loss

S. G. Georgiev, L. G. Vulkov

In recent years, honeybee losses were reported in many countries such as USA, China, Israel, Turkey, and in Europe, especially, Bulgaria. The disruption of pollination causes serious problems in economics, agriculture and ecology. In order to investigate the colony collapse, many differential equations models were proposed.
Fractional derivatives incorporate the history of the honeybee population dynamics. We study numerically the inverse problem of parameter identification in two models with Caputo and Caputo-Fabrizio differential operators. We use a gradient method of minimizing a quadratic cost functional. Numerical test with synthetic and real data from honeybee colonies of region Brestovitza are performed.

Recovering the Time-Dependent Volatility in Jump-Diffusion models from Pointwise and Nonlocal Price Observations

S. G. Georgiev, L. G. Vulkov

We propose a variational adjoint equation method for recovering the pure time-dependent volatility in a jump-diffusion framework. Diffusion-coefficient type inverse problems with local and nonlocal option price observations in Merton's and Kou's models are studied numerically. We solve approximately the nonlinear inverse problems by a gradient method of minimizing a cost functional. Numerical tests with synthetic and market data are presented.

Study the Recurrence of the Dominant Pollutants in the Formation of AQI Status Over the City of Sofia for the Period 2013-2020

I. Georgieva, G. Gadzhev

In recent years it has become possible to acquire and adapt latest models of local atmospheric dynamics WRF, transport and transformation of air pollutants CMAQ, and the emission model SMOKE. It gave an opportunity to conduct extensive studies on fully competitive modern level of the climate of atmospheric composition in the country. By using of computer simulations was created ensemble, sufficiently exhaustive and representative to make reliable conclusions for atmospheric composition typical and extreme situations with their specific space and temporal variability. The contribution of different categories of sources on the atmospheric composition has been studied. The contribution of different dynamical, chemical and aerosol processes for the atmospheric composition formation was clarified. On this base statistically significant ensemble of corresponding Air Quality indexes (AQI) was calculated, and their climate typical repeatability, space and temporal variability for the territory of the country was constructed. Similar numerical experiments with horizontal resolution of 1 km. for the city of Sofia are going on.

The AQ impact on human health and quality of life is evaluated in the terms of AQI, which give an integrated assessment of the impact of pollutants and directly measuring the effects of AQ. All the AQI evaluations are on the basis of air pollutant concentrations obtained from the numerical modelling and make it possible to revile the AQI status spatial/temporal distribution and behaviour. In Bulgaria the index, calculated in the frame of Bulgarian Chemical Weather Forecast System situated at the NIGGG–BAS.

The presented results, allow to follow highest recurrence of the indices for the whole period and seasonally, and to analyse the possible reason for high values in the Moderate and murged High and Very High bands. The meteorological conditions from one hand, the dominant pollutants from other and etc. could be reason for different possible AQI statuses.

The Semismooth* Newton Method for the Solution of Contact Problems with Tresca Friction

H. Gfrerer, J. V. Outrata, J. Valdman

An equilibrium of a linear elastic body subjected to loading and satisfying friction and contact conditions can be described by a general equation

$$0 \in f(x) + Q(x), \tag{1}$$

where $f : \mathbb{R}^n \to \mathbb{R}^n$ is single-valued and $Q : \mathbb{R}^n \rightrightarrows \mathbb{R}^n$ is a closed-graph multifunction. The new semismooth* Newton method by Gfrerer and Outrata (2019) is applied

to its numerical solution. In contrast to most available Newton-type methods for inclusions, one approximates not only the single-valued but also the multi-valued part of (1). This is performed on the basis of limiting (Morduchovich) coderivative. To ensure local superlinear convergence, one has to assume that (1) is metrically regular around and Q is semismooth* at the solution. The latter is a weakening of the classical notion of semismoothness. In the case of the Tresca friction, generalized equation (1) amounts to a variational inequality of the second kind. Multifunction Q is then a classical convex subdifferential of a function generated by the friction and contact conditions. In computational examples, finite element discretization of a full domain Ω is reduced to a contact boundary Γ_C and the semismooth* Newton method is applied only to nodes in the contact boundary. Numerical tests show that the applied method is mesh-independent, i.e., the number of iterations does not increase with the mesh size.

Mean Field Games Models Arising In Geographical Economics

D. Ghilli

We are interested in a class of spatial dynamic general equilibrium models, arising in geographical economics, that allows to take account of space heterogeneity, and of microfoundations of spatial factors allocation. We investigate the above mentioned models on the micro-level, where here each agent moves across space maximizing their own utility which also depends on the position of the other agents and on the human capital. To do this, we set the problem into the framework of Mean Field Games (MFG), whose techniques are mostly based on partial differential equations and stochastic control, and were inspired by statistical physics to study Nash equilibria in differential games with a population of infinitely many identical player.
The novelty of the models we consider lies in the dependence of the human capital on the interactions among agents (e.g. spillovers) through an aggregating term. We show the convergence of the discrete problem with N agents to the continuous model with an infinite number of agents and we study the well-posedness of the associated MFG system depending on the strength of the aggregation term. Numerical experience is provided in some particular cases.
This is a joint work with Giorgio Fabbri, Fausto Gozzi, Davide Fiaschi, Cristiano Ricci, and Giovanni Zanco.

Comparison of Different Methods for Multiple Imputation by Chain Equation

D. Grigorova, D. Tonchev, D. Palejev

Missing data is a common problem when dealing with real data from many different research fields like biostatistics, sociology, economics etc. Three types of missing data are

typically defined: missing completely at random (MCAR), missing at random (MAR), and missing not at random (MNAR). Ignoring observations with missingness could lead to serious bias and inefficiency, especially when the number of such cases is large compared to the sample size. Popular technique for solving the missing data issue is multiple imputation.
There are two general approaches for multiple imputation for dealing with the problem of missing data. One is joint modelling which draws missing values simultaneously for all incomplete variables using a multivariate distribution. The other is the fully conditional specification (FCS, also known as MICE), which imputes variables one at a time from a series of univariate conditional distributions. FCS uses a multivariate model on a single variable basis by a set of conditional densities for each incomplete variable.
In this work we consider different imputation methods under different scenarios for missingness, data dimensionality and different dependencies among the data. Our results are based on simulations performed on HPC system and show the optimal imputation methods in the different cases.

Invariant Domain Preserving Approximations for the Euler Equations with a Tabulated Equation of State

J.-L. Guermond, B. Popov, B. Clayton

We will present a construction of a first order invariant domain preserving method for the compressible Euler equations supplemented with an equation of state that is either tabulated or is given by an expression which makes solving the local Riemann problems either impossible or computationally very expensive. That is, we will assume that the pressure is coming from an oracle providing us with point values when needed. Under the assumption that the oracle provides positive pressure values for positive input for density and internal energy, we will construct a numerical method that under a standard CFL condition preserves on discrete level the invariant domain of the system: positivity of density and internal energy. Moreover, if the oracle used is a simple ideal gas law we will recover the minimum principle on the specific entropy for that case.

A Monte Carlo Method for Estimating Eigenvalues Using Error Balancing

S.-M. Gurova, A. Karaivanova

The Monte Carlo (MC) power iterations methods are successfully applied for estimating extremal eigenvalue especially those of large sparse matrices. They use truncated Markov chain simulations for estimating matrix-vector products. The iterative MC methods contain two type of errors - systematic (a truncation error) and stochastic (a probable error). The systematic error depends on the number of iterations and the stochastic error

depends on the probabilistic nature of the MC method. Balancing of these two errors has been performed for a MC method for solving systems of linear equation. But this problem is still opened when a MC method is applied for estimating eigenvalues. Eigenvalues are estimated using Markov chains with fixed length in most cases. Here we propose a new version using balancing of errors to determine the optimal length of the chain. Numerical results for estimating the largest (of the smallest) eigenvalue are also presented.

BURA-Based Fractional in Space Diffusion-Reaction Approximation Error Analysis

S. Harizanov, N. Kosturski, I. Lirkov, S. Margenov, Y. Vutov

This talk is devoted to the experimental analysis of the behavior of the univariate error $E_{q,k,\alpha}$, related to the (k,k) best uniform rational approximation (k-BURA) $r_{q,k,\alpha}(t)$ of the function $t^\alpha/(1+qt^\alpha)$ on the unit interval. More precisely, for given $q \geq 0$, $\alpha \in (0,1)$, $k \in \mathbb{N}$, we define

$$r_{q,k,\alpha}(t) := \operatorname*{argmin}_{r \in \mathcal{R}(k,k)} \left\| r(t) - \frac{t^\alpha}{1+qt^\alpha} \right\|_{C[0,1]}, \quad E_{q,k,\alpha} := \left\| r_{q,k,\alpha}(t) - \frac{t^\alpha}{1+qt^\alpha} \right\|_{C[0,1]}.$$

In our previous works it has been established that $E_{q,k,\alpha}$ is an upper bound for the ℓ_2 approximation error of a BURA-based numerical solver for the fractional in space discretized diffusion-reaction problem $\mathbf{u} = (\mathbb{A}^\alpha + q\mathbb{I})^{-1}\mathbf{f}$, where $\mathbb{A}$ is an SPD matrix with spectrum in $[1,+\infty)$, and its fractional power is derived with respect to spectral decomposition.
We will show that

$$E_{q,k,\alpha} = C(q,k,\alpha)\frac{E_{0,k,\alpha}}{1+q},$$

with $C(q,k,\alpha)$ strictly monotonically increasing with respect to all three arguments. Furthermore, for a fixed $k = k_0$ we will investigate the limit $\lim_{\alpha\to 1, q\to\infty} C(q,k_0,\alpha)$ and will provide numerical evidence that it should be finite. Therefore, since $E_{0,k,\alpha} \sim 4^{1+\alpha}|\sin(\pi\alpha)|e^{-2\pi\sqrt{k\alpha}}$, we conjecture that $E_{q,k,\alpha} = \mathrm{O}(q^{-1})e^{-2\pi\sqrt{k\alpha}}$.

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Reduced Sum Implementation of the BURA Method for Spectral Fractional Diffusion Problems

S. Harizanov, N. Kosturski, I. Lirkov, S. Margenov, Y. Vutov

The presented results concern the numerical solution of spectral fractional diffusion problems in the form $\mathcal{L}^\alpha u(x) = f(x)$, where $\mathcal{L}$ is a selfadjoint elliptic operator in a bounded

domain $\Omega \subset I\!R^d$, $d \in \{1, 2, 3\}$, and $\alpha \in (0, 1]$. The finite difference approximation of the problem leads to the system $A^\alpha \mathbf{u} = \mathbf{f}$, where A is a sparse, symmetric and positive (semi)definite matrix, and A^α is defined by its spectral decomposition. In the case of finite element approximation, A is symmetric with respect to the energy dot product associated with the mass matrix. The BURA method is introduced by the best uniform rational approximation of degree k of t^α in $[0, 1]$, denoted by $r_{\alpha,k}(x)$. Then the approximation $\mathbf{w} \approx \mathbf{u}$ is expressed in the form $\mathbf{w} = -b_0\mathbf{f} - \sum_{i=1}^{k} b_i(A + c_i I)^{-1}\mathbf{f}$, $c_i > 0$, thus requiring solving of k auxiliary linear systems with sparse and symmetric positive definite matrices. The BURA method has almost optimal computational complexity, assuming that some optimal solution method is applied to the involved auxiliary linear algebraic systems. We have used the BoomerAMG implementation of the algebraic multigrid method in the framework of a preconditioned conjugate gradient (PCG) iterative solver.
The theoretical analysis shows that the first part of c_i become extremely large. This is stronger expressed for smaller α and larger k. The presented numerical tests show that in this case the condition number of $A + c_i$ is practically equal to one. Obviously, such systems do not need preconditioning. The next question is if we can replace the solution of related systems by multiplication of $\mathbf{f}$ with b_i/c_i. This is the motivation to consider a reduced sum implementation of BURA. The properties of the proposed algorithm are studied. Representative numerical tests are presented.

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Graph Laplacians: Algorithms and Applications

X. Hu

Many practical applications involve a rich spectrum of networks, which are modeled by graphs. In many of these applications, such as social, biological, or energy networks, the solution of large-scale graph Laplacians is a key ingredient of the computational model. Therefore, developing effective algorithms for such systems is an important and challenging task in these scientific computing applications. In this talk, several recent advancements for solving graph Laplacians are introduced, including the design of multi-level graph sparsifiers and a posteriori error estimation. Such methods are then applied to various network applications, including protein-protein interaction networks and brain modeling, to demonstrate the efficiency of the algorithms. Finally, if time permits, a generalization to Hodge Laplacians on graphs and their applications in statistical and scientific machine learning will be discussed.

A Posteriori Error Estimates for Solving Graph Laplacians

X. Hu, K. Wu, L. Zikatanov

We study a posteriori error estimators which aid multilevel iterative solvers for linear sys-

tems with graph Laplacians. In earlier works, such esti- mates were computed by solving global optimization problems, which could be computationally expensive. We propose a novel strategy to compute these estimates by constructing a Helmholtz decomposition on the graph based on a spanning tree and the corresponding cycle space. To compute the error estimator, we solve efficiently the linear system on the spanning tree, and then we solve approximately a least-squares problem on the cycle space. As we show, such an estimator has a nearly-linear computational complexity for sparse graphs under certain assumptions. Numerical experiments are presented to demonstrate the efficacy of the proposed method.

Multi-Lingual Emotion Classification using Convolutional Neural Networks

A. Iliev, A. Mote, A. Manoharan

Emotions play a central role in human interaction. Interestingly, different cultures have different ways to express the same emotion, and this motivates the need to study the way emotions are expressed in different parts of the world to understand these differences better. This paper aims to compare 4 emotions namely, anger, happiness, sadness, and neutral as expressed by speakers from 4 different languages (Canadian French, Italian, North American English and German - Berlin Deutsche) using modern digital signal processing methods and convolutional neural networks.

On Pore Scale Simulation of Reactive Flows in Porous Media

O. Iliev, T. Prill, P. Toktaliev

Reactive flows in porous media are an essential component of many technological and environmental problems. The reactions take place at pore or even surface of pore scale, therefore detailed study at this scale is needed in order to better understand the processes. Pore scale simulation for such flows is a challenging numerical task, especially in the presence of geometrical and chemical heterogeneity, complex chemical reactions, multirate reactions, etc. The current talk will elaborate on the recent developments in this area by a team in Fraunhofer ITWM, will review the achievements and will state the open problems.

On to Parallel MLMC for Stationary Single Phase Flow Problem

O. Iliev, N. Shegunov, P. Armyanov, A. Semerdzhiev I. Christov

Many problems that incorporate uncertainty, at some point, usually require solving a Stochastic Partial Differential Equation. Fast and efficient methods for solving such

equations are of particular interest for Computational Fluid Dynamics(CFD) and more precisely to problems involving porous medium flows. It is believed with the advances of the HPC systems a breakthrough is possible. One of the main limitations for advances in this area is the lack of fast methods that are capable of simulating realistic problems. For example, suppose a simulation of an underground water flow in an area of hundreds of square km. The usual go-to method for such simulations is the Multilevel Monte Carlo method. This is a more general form of the well know class of Monte Carlo computational methods. It relies on repeated random sampling on different levels. The approach is to sample not only from the SPDE but also from approximations of the SPDE on coarser grids to obtain numerical results. By this, MLMC overcomes the slow convergence rate of the classical MC methods. The problem of finding optimal processor distribution is considered NP-complete. In this paper, a stationary single-phase flow through a random porous medium is regarded as a model problem. Although a simple model, it is well-established problem in the field, that shows well the computational changes involving MLMC simulation. For this model different dynamic scheduling strategies exploiting three-layer parallelism are examined. The considered schedulers consolidate the sample to sample time differences. In this way, more efficient use of computational resources is achieved.
The computational MLMC model requires three main steps: a correlated random number generator for the permeability field, a numerical scheme for discretization of the PDE, and a coarse grain method that approximates the solution on the different levels. To construct the model is done in the following way: The Circulant Embedding approach is used as a random generator, the cell-centered finite volume method for numerical discretization, and simplified renormalization as a coarse grain approach for the MLMC.

Computational Study of *Helix Aspersa* Mucus Peptides in Complex with a Model Bacterial Membrane

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

In the last years, antibacterial, antiviral and even anticancer activity of bioactive substances of garden snails *Helix aspersa* and *Helix lucorum* have been proven in a number of clinical studies. The AMPs' antibacterial activity is thought to be based on their cationic and amphiphilic nature, which enables them to interact with negatively charged bacterial surfaces and membranes, thus causing membrane disruption or altering metabolic processes. Thus, a relation can be established between cell membrane permeability under the action of AMPs and their antibacterial activity.
We discuss a metadynamics-based protocol aiming at a possibly exhaustive sampling of the conformation space of the AMP–membrane complex. The model membrane is constructed to resemble the *E. Coli* membrane: asymmetric, with POPE (neutral) and POPG (negatively charged) phospholipids in ratios 85/15 and 70/30 in the external, resp. internal layer. This enhanced sampling technique provides information about the multidimensional free energy surfaces in terms of appropriate collective variables. The influence of the collective variables choice is exemplified by two different sets of collective variables

the peptide/membranbe center-of-mass distance and the centre-of-mass distance for a up to three charge groups.

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Solving Systems of Polynomial Equations - a Tensor Approach

M. Ishteva, P. Dreesen

Polynomial relations are at the heart of mathematics. The fundamental of solving polynomial equations shows up in a wide variety of (applied) mathematics, science and engineering problems. Although different approaches for solving systems of polynomial equations have been considered in the literature, the problem remains difficult and requires further study.

We propose a solution based on tensor techniques. In particular, we build a partially symmetric tensor from the coefficients of the polynomials and decompose this tensor with the canonical polyadic decomposition. Due to the partial symmetry, a structured version of the canonical polyadic de-composition is needed. The factors of the decomposition can then be used for building systems of linear equations, from which we find the solutions of the original system.

In this paper we present our new approach and illustrate it with a number of examples. Although this approach is not applicable for solving an arbitrary system of polynomial equations, it is applicable to a large class of sub-problems. Future work includes comparing the proposed method to existing methods and extending the class of subproblems, for which the method can be applied.

Behaviour and Scalability of the Hydrostatic and Non-Hydrostatic Cores of RegCM Multiscale Simulations on High Performance Computing Platforms

V. Ivanov, G. Gadzhev

The RegCM is a regional climate model used in many studies. There are simulation runs in different domains, time-periods, and regions in the world on all continents. The research works in our group, are related to the historical and future climate, and its influence on the human sensation over South-east Europe. We used the model versions

4.4 and 4.7. The main model components are the initial and boundary condition module, the physics processes parametrization module, and the dynamical core. Concerning the last one, we used the default one the hydrostatic option corresponding to the MM5 model dynamical core. We run simulations with different combinations of parametrization schemes on the Bulgarian supercomputer Avitohol. The newer versions of the model have an additional option for using a non-hydrostatic dynamical core, which allows model simulations to be done with finer resolutions. Increasing the temporal and spatial resolution leads to increasing the requirements of the computational resources. The running of model simulations with different input configurations depends highly on the available computing resources. Several main factors influence the simulation times and storage requirements. They could vary much depending on the particular set of input parameters, domain area, land cover, processing cores characteristics, and their number in parallel processing simulations. The objective of that study is to analyze the RegCM model performance with hydrostatic core, and non-hydrostatic core, on the High-Performance Computing platform Avitohol.

Extreme Scale Computations of Transitional Regime in Physiologic Flows

K. Jain

Presence of turbulent like fluctuations in physiological flows has been known for a long time. Recent computational studies found such flow regime in blood flow in aneurysms, flow in the left ventricle as well as the oscillatory cerebrospinal fluid (CSF) flow in the spinal canal. The physical, and physiological significance of such a flow regime remains questionable thereby raising a question whether numerical methods should be appropriately chosen and resolved to characterize such phenomena. Furthermore, characterization of such a flow regime requires development and validation of massively parallel simulation frameworks that are capable to capture intricate dynamics of flow in such regimes.
We developed a massively parallel framework, Musubi based on the lattice Boltzmann method (LBM). On one hand we report simulations of transitional flow in the FDA nozzle at throat Reynolds number of 2000 and 2500 that were executed on 304128 CPUs (the whole system) of the SuperMUC-NG petascale system installed in Munich, Germany. The meshes were discretized with up to 2.8 billion cells. The simulations demonstrate reasonable agreement with the experiments of the FDA and provide insights into the detailed physics of flow addressing questions like the role of resolutions in predicting the jet breakdown locations.
Further, we explore the physics of the motion of purely oscillatory flow in stenosed vessels exploring the critical Reynolds number at which such a flow transitions to turbulence. We demonstrate that the zero mean nature of oscillatory flows has a stabilizing effect on the flow field, which leads to an elevation in critical Reynolds number for flow transition compared to a uni-directional pulsatile flow. The simulations were conducted using 28800 cores of the Hazel Hen system installed in Stuttgart, Germany. In the presentation, the physics of such flows, performance of the code and the need for such large scale

computations will be discussed.

Applications of Strong Regularity to Optimal Control of Parabolic Partial Differential Equations

N. A. Jork

The talk will discuss sufficient conditions for strong metric regularity and subregularity properties of the solution mapping of optimal control problems of parabolic PDEs. These properties have numerous applications to error analysis of numerical methods and for obtaining Lipschitz dependence of the solution on parameters or perturbations. In particular, the talk will focus on Tikhonov regularization of non-coercive problems. This is especially relevant to optimal control problems, where the L^1-norm of the control appears in the objective functional (instead of the L^2-norm). Such problems are recently a subject of intense investigation due to various applications, including sparse control problems.

Optimizing Numerical Methods Using Machine Learning

A. Katrutsa, I. Oseledets

One of the promising applications of modern machine learning methods is to optimize existing algorithms. Instead of putting generic deep neural network black-boxes, one can look at classical iterative methods as compositions of simple functions, amenable to optimization. We show the applicability of this approach to different problems, including multigrid and BPX preconditioners.

Quantum Effects on 1/2[111] Edge Dislocation Motion in Hydrogen-Charged Fe from Ring-Polymer Molecular Dynamics

I. Katzarov, N. Ilieva, L. Drenchev

Hydrogen-influenced change of dislocation mobility is a possible cause of hydrogen embrittlement (HE) in metals and alloys. A comprehensive understanding of HE requires a more detailed description of dislocation motion in combination with the diffusion and trapping of H atoms. A serious obstacle towards the atomistic modelling of a H interstitial in Fe is associated with the role nuclear quantum effects (NQEs) might play even at room temperatures, due to the small mass of the proton. Standard molecular dynamics (MD) implementations offer a rather poor approximation for such investigations as the nuclei are considered as classical particles. Instead, we reach for *Ring-polymer MD*

(RPMD), the current state-of-the-art method to include NQEs in the calculations, which generates a quantum-mechanical ensemble of interacting particles by using MD in an extended phase space.
Here we report RPMD simulations of quantum effects on 1/2[111] edge dislocation motion in H charged Fe within the open-source code i-PI. The simulations results indicate that H atoms are more strongly confined to dislocation core and longer relaxation time is necessary for the screw dislocation to break away from the H atmosphere. The stronger interaction between dislocation and H atoms trapped in the core, resulting from NQEs, leads to formation of jogs along the dislocation line which reduce edge dislocation mobility in H charged Fe.

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Fitted Finite Volume Method for an Unsaturated Flow Problem with Space Degeneration

M. N. Koleva, L. G. Vulkov

Over the past decade unsaturated flow has become one of the most important and active topics of the research. A common used models in the theory of subsurface flow is the Richards' equation. It can be written in a number of forms, namely the water content, mixed water content and capillary head form, and the head form. In the present work, we consider a slightly modification of the classical Richards' equation of water content on time in porous medium. Existence and uniqueness properties of the solution are discussed.
First we apply time discretization and linearize the obtained nonlinear problem. Then, we develop fitted finite volume method for solving the model problem. We show that the method is efficient in the case of degenerate and discontinuous permeability. We present and discuss numerical results.

On Red Refinements of Tetrahedral Meshes

S. Korotov

Red refinement of simplicial meshes is one of the most popular techniques for mesh generation and adaptivity when the finite element method is used.

In the talk we shall discuss various regularity issues for different versions of the red refinement in the context of tetrahedral (and higher–dimensional) meshes. A number of very recent own results will be presented.

On the Small-Time Local Controllability

M. I. Krastanov, M. N. Nikolova

The small-time local controllability of a nonlinear control system with bounded controls is studied. The gap between the existing necessary and sufficient controllability conditions is briefly discussed. A general necessary controllability condition is shown under natural assumptions. Moreover, a sufficient controllability condition for polynomial systems of second degree is presented. The proposed approach for studying the local properties of the corresponding reachable set is based on the Campbell-Baker-Hausdorf formula. Different examples illustrate the applicability of the obtained results.

Bounded Linear-Quadratic Optimal Control Problem in the Presence of Disturbances

M. Krastanov, R. Rozenov, B. Stefanov

A linear-quadratic optimal control problem with convex control constraints is studied on an infinite-time horizon in the presence of disturbances. A numerical approach for solving this problem is proposed. This approach is based on solving a suitable algebraic Riccati equation and using the Pontryagin maximum principle. Numerical examples illustrate the proposed approach.

A New Framework for the Stability Analysis of Perturbed Saddle-Point Problems and Applications in Poromechanics

J. Kraus

In this talk we prove a new abstract stability result for perturbed saddle-point problems based on a norm fitting technique. We derive the stability condition according to Babuška's theory from a small inf-sup condition, similar to the famous Ladyzhenskaya-Babuška-Brezzi (LBB) condition, and the other standard assumptions in Brezzi's theory, in a combined abstract norm. The construction suggests to form the latter from individual *fitted* norms that are composed from proper seminorms.
This abstract framework not only allows for simpler (shorter) proofs of many stability results but also guides the design of parameter-robust norm-equivalent preconditioners.

These benefits are demonstrated with several examples arising from different formulations of Biot's model of consolidation.
This is joint work with Maria Lymbery and Fadi Philo from the University of Duisburg-Essen and Qingguo Hong from The Pennsylvania State University.

On The Stability of Time-Discrete Systems Arising from Second-Order Implicit Time-Stepping Schemes Applied to Dynamic Multiple Network Poroelasticity Models

J. Kraus, M. Lymbery, F. Philo

The equations governing the interaction of the solid and fluid media were first established for quasi-static phenomena.The quasi-static model was first established by Biot in 1941, who extended it later to describe dynamic phenomena. Dynamic multiple-network poroelastic theory (MPET) generalizes Biots consolidation model.
We analyze the stability properties of the time-discrete systems arising from second-order implicit time stepping schemes. They are applied to the variational formulation of the MPET model. By introducing parameter-dependent norms, we proof an inf-sup condition with a constant that is independent of all model parameters. This leads to existence and uniqueness of the solution. The norms in which these results hold are the basis for parameter-robust preconditioners. The result is supported by a numerical example for a dynamic Biot model.

The Universality of Deep Neural Networks: An Expressivity Analysis

G. Kutyniok

We currently witness the impressive success of deep neural networks in real-world applications, ranging from autonomous driving over game intelligence to the health care sector. At the same time, deep learning-based methods have a similarly strong impact on the entire range of science, often replacing classical model-based methods to solve mathematical problems such as inverse problems or partial differential equations in the state of the art. However, despite this outstanding success, most of the research on deep neural networks is empirically driven and a mathematical foundation is largely missing.
In this talk, after a brief introduction into theoretical aspects of deep learning, we will analyze neural networks from an expressivity viewpoint. Our main focus will be on theoretically analyzing the ability of deep neural networks to universally perform at least as good as most approximation schemes, e.g., wavelet or shearlet approximation, while in addition being able to beat the curse of dimensionality in applications such as parametric partial differential equations. We will also present diverse numerical examples showing the effectiveness of such deep learning-based methods.

Stabilizability in Optimization Problems

A. C. Lai, M. Motta

We review some recent results concerning the global asymptotic stabilizzabiity of control systems, when a cost is also considered. We extend the notions of Sample and Euler stabilizability to a wide class of unbounded control systems, also including nonlinear control-polynomial systems. We then take into account the associated cost and we provide sufficient conditions for the existence of a stabilizing feedback K, possibly unbounded around the target, such that all the corresponding sampling and Euler solutions have costs bounded above by the same continuous state-dependent function. Such conditions are based on the existence of a special Control Lyapunov Function, which also provide an explicit construction of the required feedback K.

Adaptive Space-Time Finite Element Solvers for Parabolic Optimal Control Problems

U. Langer, O. Steinbach, F. Tröltzsch, H. Yang

We consider tracking-type optimal control problems constrained by linear parabolic partial differential equations with distributed Here, space-time finite element methods on unstructured simplicial meshes are especially suited, since the reduced optimality system couples two parabolic equations for the state and adjoint state that are forward and backward in time, respectively. The analysis of the reduced optimality system and discretization error estimates are based on Banach-Nečas-Babuška-Azizs theorems. In contrast to time-stepping methods, one has to solve one large-scale linear algebraic system of finite element equations. The solution of this system provides continuous finite element approximations to the state and the adjoint state in the whole space-time cylinder at once. Full space-time adaptivity, parallelization, and matrix-free implementations are very important techniques to overcome the increased memory requirement of space-time finite element methods. Fast parallel solvers are another important ingredient of efficient space-time methods. We first consider the standard L_2 regularization, and then compare it with sparse optimal control techniques and a new energy regularization. The numerical results confirm the convergence rate estimates in the case of uniform refinement, the efficiency of the adaptivity procedure proposed, and they clearly show the effects of different regularization techniques.
The space-time approach proposed in the talk can be extended to other optimal control problems like partial control, boundary control, initial date control, partial observation, terminal observation, but also to non-linear parabolic state equations and box constraints imposed on the control.

On Parameter-Robust Finite Element Methods for Multiple-Network Poroelasticity Problems

J. Lee

Numerical methods for multiple-network poroelasticity (MPET) models are of great research interest recently. We discuss preconditioning techniques of finite element methods which are robust for the fluid exchange coefficients of MPET models. This is a joint work with Kent-Andre Mardal, Marie E. Rognes, Eleonora Piersanti, and Travis B. Thompson.

Space-Time Error Indicator for Biot's Consolidation Model

Y. Li, L. T. Zikatanov

In this talk, we present space-time posteriori error estimates of discretizations for Biot's consolidation model, based on implicit Euler method in time and mixed finite element in space. The error indicator is shown to be an upper and lower bound of the space-time discretization error. It also leads to a new error estimator for the heat/Darcy equation in mixed form.

Effluent Recirculation for Contaminant Removal in Constructed Wetlands under Uncertainty: A Stochastic umerical Approach Based on Monte Carlo Methodology

K. Liolios, G. Skodras, K, Georgiev, I. Georgiev

The problem of the alternative operational technique concerning effluent recirculation in Horizontal Subsurface Flow Constructed Wetlands (HSF CW) to remove pollutants under uncertainty is investigated numerically, in a stochastic way. Uncertain-but-bounded input-parameters are considered as interval parameters with known upper and lower bounds. This uncertainty is treated by using the Monte Carlo method. A typical pilot case of an HSF CW concerning Biochemical Oxygen Demand (BOD) removal is presented and numerically investigated. The purpose of thestudy is to compare the relevant numerical results with the available experimental ones, and so the effectiveness and the reliability of the proposed stochastic approach to be proven.

On Pontryagin Type Maximum Principle for Budget-constrained Infinite Horizon Optimal Control Problems

V. Lykina

In this paper we consider a class of infinite horizon optimal control problems with budget constraints. The dynamics of the controlled system is assumed to be linear in control. Further, the optimal control problem as a whole is considered in the framework of weighted functional spaces approach. Therefore, we choose a weighted Sobolev space and a weighted Lebesgue space as the state and the control spaces respectively. The objective as well as the budget constraint also contain weight functions. For the obtained class of problems we prove necessary optimality conditions in form of Pontryagin Type Maximum Principle. The latter contain transversality condition in form of an integral inclusion as well, whereby the proof is based on the Hahn-Banach separation theorem. The applicability of theoretical results is shown by means of an example.

Simulation of Fluid Transport in the Human Brain: A Comparison of Discretizations and Solvers

M. Lymbery

In this talk we compare discretizations and solvers for simulations of fluid transport in the brain. We consider the multiple-network poroelastic theory (MPET) model which is commonly used to describe mechanical deformation and fluid flow in the cerebral environment. The networks of interest consist of the arterial, venous, capillary and extracellular fluid networks.

We study several finite element (FE) approximations of the three-field formulation of the MPET model where the primary physical variables are the parenchymal tissue displacement, the seepage velocities and scalar pore pressures of the four fluid compartments; namely, we consider the $\mathrm{P}_{\ell+1}/\mathrm{P}_\ell/\mathrm{P}_\ell$, the stabilized with bubble functions $\mathrm{P}_1^{\mathrm{stab}}/\mathrm{RT}_0/\mathrm{P}_0^{\mathrm{dc}}$ and the $\mathrm{BDM}_\ell/\mathrm{RT}_{\ell-1}/\mathrm{P}_{\ell-1}^{\mathrm{dc}}$ FE discretizations, with P_ℓ, BDM_ℓ and RT_ℓ denoting the space of full piecewise polynomials and the spaces of Brezzi-Douglas-Marini and Raviart-Thomas of order ℓ, respectively.

We show that these discretizations yield quite different numerical results when used for problems with boundary layers of a brain domain and we discuss the causes of this phenomenon. The talk finishes with comparison of the computational efficiency of several iterative solvers for the arising linear systems pointing out advantages of hybridization techniques.

This is joint work with Johannes Kraus and Kevin Osthues from the University of Duisburg-Essen and Philip Lederer and Joachim Schöberl from the Technical University of Vienna.

A Multiscale Approach To Fatigue-Damage Modeling In Short-Fiber Reinforced Plastics

N. Magino, H. Andrä, F. Welschinger, R. Müller, M. Schneider

Short fiber reinforced composites are of increasing interest in engineering science. To ensure a safe use in industrial applications undergoing complex operational loads, the prediction of their fatigue behavior is essential. The fiber distribution inside an engineering component greatly depends on the injection molding process. Typically, one expects a multitude of possible fiber orientations that vary significantly throughout the (macroscale) component. In an engineering context, direct computations resolving the fibers are numerically not feasible.
We approach this issue by a multiscale method: On the microscale we use an isotropic compliance-based damage model formulated in logarithmic cycle space for the matrix. The choice of a convex free energy functional enables a consistent derivation of macroscopic properties based on representative volume elements. Upon precomputations for a finite set of fiber orientations, we build a database via model order reduction. Due to our choice of the material model, the free energy potential can not be expressed as polynomial in internal variables and strains. To obtain a convenient formulation for model order reduction we thus reformulate the model in terms of stress and internal variables. On the macroscale we access the precomputed database and can efficiently perform computations on engineering problems.
We report on recent progress and present numerical tests.

A Nonnegative Tensor-Train Based Method for the Smoluchowski Coagulation Equation

G. Manzini

In this talk, we present a numerical method for the time-dependent multicomponent Smoluchowski coagulation equation, where the different components are represented as independent space dimensions. The algorithm relies on a predictorcorrector time-stepping scheme and the high-dimensionality of the problem is addressed by using suitable nonnegative tensor-train formats. To this end, we discretize the component densities and the coagulation kernel as grid functions evaluated at the nodes of a multidimensional grid, which are practically stored and managed by the numerical algorithm through special low-parametric representations. This approach makes it possible to reduce the computational complexity to $O(d^2 N log N)$, where is the number of nodes per axis in the space grid and d is the number of components. Numerical experiments are carried out to assess the performance of the method.

Random Lift Of Set-Valued Maps And Applications

A. Marigonda

We discuss some preliminary results about the lifting of set-valued maps defined between Polish spaces to set-valued maps defined between the corresponding spaces of probability measures. In particular, we are interested to establish conditions granting that some relevant properties (for instance semicontinuity, compactness of the images, Lipschitz continuity,...) of the original set-valued maps are conserved also in the lifted map.
The main motivation of the study is the dynamics and the control of multi-agent systems, where the macroscopical trajectory can be seen as the lift of the solution set-valued map of a differential inclusion expressing the microscopical dynamics of the agent, however our results can be extended to more general set-valued maps of agent trajectories provided that they enjoys some properties.

Joint work with: Rossana Capuani (University of Verona) and Michele Ricciardi (University of Verona).

Minimization of Energy Functionals via the Finite Element Method in MATLAB

C. Matonoha, A. Moskovka, J. Valdman

Many problems in science and engineering have their mathematical formulation which leads to solving an operator equation

$$Au = f\,, \qquad u \in M\,, \quad f \in H\,, \tag{1}$$

where H is a Hilbert (or Banach) space, M is a subspace of H, u is a solution of (1) and A is an operator on M. In particular, we will focus on differential operators. There are a lot of methods for solving (1) and one of them is the so called variational approach which is based on finding the minimum of corresponding energy functional. In our text we represent the variational principle for solving some particular problems using a finite elements method (FEM) for discretization of energy functionals. Minimization procedures of energy functionals require the knowledge of a gradient. If an exact gradient form is not available or difficult to compute, a numerical approximation can be assembled locally. The key feature is the sparsity of Hessian matrix which significantly affects the time and memory demands of evaluations.
We firstly introduce a simple minimization problem taken from section on Minimization with Gradient and Hessian Sparsity Pattern of MATLAB documentation. Then we implement our techniques on solving p-Laplace equation in two space dimensions.
In our codes we emphasize an effective gradient computation via matrix operations (the so called vectorization technique). Discretized functionals are minimized using an implemented functions in MATLAB which include Trust-region methods and which efficiency can be significantly improved by specifying the sparsity of Hessian matrix. In particular,

in our codes we operate with triangle elements on rectangle sets, however, these techniques can be used for more general sets and arbitrary discretization via finite elements.

Data Driven Enhanced Methods For Terahertz Tomography

C. Meiser, T. Schuster, A. Wald

In terahertz tomography the aim is to compute the complex refractive index

$$\tilde{n}(x) = n(x) + i\kappa(x), \quad x \in \Omega$$

with the index of refraction $n(x)$ and the absorption coefficient $\kappa(x)$ of a material from measurements which consist of reflections and transmissions of electromagnetic waves in the range of 0.1-10 THz. This is an inverse imaging problem where the underlying mathematical problem is associated with Maxwell's equations and simplifications thereof. One idea is to neglect the wave character and use geometric optics which leads to the eikonal equation as mathematical model. The eikonal equation results as a high frequency approximation of the Helmholtz equation and, more generally, of the wave equation. In that sense we deal with the inverse problem of computing the refractive index $n(x)$ from time-of-flight measurements. Applying Landweber's method we solve the nonlinear partial differential equation for the forward operator in every step, but also need to compute the adjoint operator of the Frchet derivative. When talking about inverse problems deep learning and neural network based algorithms are an emerging field. Using training data which, e.g., consist of the refractive index and associated measure data, to train a neural network, we accelerate the evaluation of the forward operator, i.e. the solution of the eikonal equation, significantly compared to standard techniques such as marching schemes. This also leads to a more efficient solution of the inverse problem itself.
Further, we consider a data driven anomaly detection algorithm in in-line monitoring. We focus on plastic for which the terahertz radiation is perfectly suited, and propose a density based technique to detect automatically anomalies in the measured data of the radiation. Numerical results will be presented.

binMeta: a New Java package for Meta-heuristic Searches

A. Mucherino

We present the new binMeta package, a Java package for the development of meta-heuristic searches for combinatorial optimization under a common interface. Several combinatorial optimization problems arising in real-life applications have been proved to belong to the class of NP-hard problems, for which a deterministic algorithm for their solution cannot be devised. We focus therefore on generic (i.e. not focusing on any special class of problems) meta-heuristic approaches for the solution of combinatorial

optimization. Although we are aware that this is not the first attempt to develop one unique tool implementing several meta-heuristics, binMeta is a tool whose development has been following some special particular guidelines, which can potentially enhance its applicability and imply a large use. Our main development guidelines are as follows.

- *We keep it simple*: We mainly select meta-heuristic searches that are able to deliver good-quality solutions with relatively simple implementations; also, every different search phase is, as far as this is possible, isolated in a separated Java method, so that it can potentially be reused in other implementations.
- *Low-level representation of solutions*: In order to restrict our searches to a finite discrete subset of possible solutions, we use a "low level" representation of the problem solutions, encoded as a bit string. This approach allows us to compact the solution representation in the memory space and, more importantly, it allows us to reduce the solution's degrees of freedom to the minimum values.
- *High-level organization of the Java classes*: The classes in the Java package are conceived with the idea to satisfy a high "inter-connection" level. As for example, a meta-heuristic search itself can be seen as a combinatorial optimization problem in our package, where its own parameters can play the role of decision variables.

The initial versions of the binMeta package can be found on GitHub.

Model Reduction for Large Scale Systems

M. Ohlberger

Projection based model order reduction has become a mature technique for simulation of large classes of parameterized systems. However, several challenges remain for problems where the solution manifold of the parameterized system cannot be well approximated by linear subspaces. While the online efficiency of these model reduction methods is very convincing for problems with a rapid decay of the Kolmogorov n-width, there are still major drawbacks and limitations. Most importantly, the construction of the reduced system in the offline phase is extremely CPU-time and memory consuming for large scale and multi scale systems. For practical applications, it is thus necessary to derive model reduction techniques that do not rely on a classical offline/online splitting but allow for more flexibility in the usage of computational resources. A promising approach with this respect is model reduction with adaptive enrichment. In this talk we investigate (localized) model reduction with adaptive basis enrichment for the solution of multiscale problems and large scale PDE constrained parameter optimization.

A New Family of Hybridized Discontinuous Galerkin/Hybrid Mixed Discretizations for Multiple Network Poroelasticity

K. Osthues

We consider the quasi-static multiple network poroelastic theory (MPET) model in a three-field formulation, the unknown physical quantities of interest being the displacement $\mathbf{u}$ of the solid matrix, the seepage velocities $\mathbf{v}_i$ and pore pressures p_i of the n networks, $i = 1, \ldots, n$. In order to conserve fluid mass we propose a hybridized discontinuous Galerkin method for the elasticity subproblem combined with a mixed method for the flow subproblems which are also handled by hybridization. In addition, this allows the elimination of the seepage velocities by a static condensation process.
As a result, the system to be solved only contains degrees of freedom for $\mathbf{u}$ and p_i, $i = 1, \ldots, n$, thereby making this approach especially favourable for higher-order approximations. Algorithmic aspects are discussed and a stability analysis is presented which yields well-posedness of the discrete problem, optimal error estimates and parameter-robust preconditioners, the latter providing a key tool for developing uniformly convergent iterative solvers. The cost-efficiency of the proposed approach is demonstrated on three-dimensional test examples.
This is joint work with Johannes Kraus and Maria Lymbery from the University of Duisburg-Essen and Philip Lederer and Joachim Schöberl from the Technical University of Vienna.

Sensivitity Study of Large-Scale Air Pollution Model Based on Modifications of the Latin Hypercube Sampling Method

T. Ostromsky, V. Todorov, I. Dimov, R. Georgieva, Z. Zlatev

We discuss a systematic approach for sensitivity analysis studies in the area of air pollution modelling. Different parts of the large amount of output data, produced by the model, were used in various practical applications, where the reliability of this data should be properly estimated. Another reason to choose this model as a case study here is its sophisticated chemical scheme, where all relevant chemical processes in the atmosphere are accurately represented. We study the sensitivity of concentration variations of some of the most dangerous air pollutants with respect to the anthropogenic emissions levels and with respect to some chemical reactions rates.
A comprehensive experimental study of Monte Carlo algorithm based on modifications of the Latin Hypercube Sampling for multidimensional numerical integration has been done. Samplings with different seeds has been analyzed. We use a division of the distribution of each variable into equiprobable intervals. The values obtained for each variable are paired randomly. This comparison has been made for the first time for sensitivity analysis of UNI-DEM. The algorithms have been successfully applied to compute global Sobol

sensitivity measures corresponding to the six chemical reactions rates and four different groups of pollutants.
The numerical tests will show that the stochastic algorithms under consideration are efficient for the multidimensional integrals under consideration and especially for computing small by value sensitivity indices. Clearly, the progress in the area of air pollution modeling, is closely connected with the progress in reliable algorithms for multidimensional integration.

A New Algorithm for the LQR Problem with Partially Unknown Dynamics

A. Pacifico, A. Pesare, M. Falcone

We consider a Linear Quadratic Optimal Control problem with partially unknown dynamics, using a numerical approach closely related to Reinforcement Learning. We deal with a new model-based online algorithm to obtain an approximation of the dynamics *and* the control at the same time during a single simulation.
The uncertain knowledge of the dynamics is represented as a probability distribution over the set of possible dynamics, which are matrices in the linear case. At each step, the control is chosen according to the present knowledge of the dynamics, solving the Riccati equation. Then the probability distribution is updated according to the prior knowledge and the observed behavior of the system. This update is obtained by means of Bayesian formulas to produce a new description of the dynamics that is used in the next step.
We present some numerical tests based on this approach, showing that the algorithm is able to stabilize the system in all of them.

Numerical Parameter Estimates of Beta-uniform Mixture Models

D. Palejev

When analyzing biomedical data, researchers often need to apply the same statistical test or procedure to many objects resulting in a multiple comparison setup. A portion of the tests are statistically significant, their unadjusted p-values form a spike near 1 and as such they can be modeled by a suitable Beta distribution. The unadjusted p-values of the non-significant ones are drawn form a uniform distribution in the interval [0, 1]. Therefore the set of all unadjusted p-values can be represented by a Beta-uniform mixture model. Finding the parameters of that model plays an important role in estimating the statistical power of the subsequent Benjamini-Hochberg correction for multiple comparisons. To empirically investigate the properties of the parameter estimation procedures we carried out a series of computationally intensive numerical simulations on a high-performance computational facility. As a result of these simulations, in this article we present a model for the the asymptotic convergence of the parameter estimates when increasing the number of tests under different conditions for the parameters of the mixture.

Boolean Hierarchical Tucker Networks on Quantum Annealers

E. Pelofske, G. Hahn, D. O'Malley, H. Djidjev, B. Alexandrov

Quantum annealing is an emerging technology with the potential to solve some of the computational challenges that remain unresolved as we approach an era beyond Moore's Law. In this work, we investigate the capabilities of the quantum annealers of D-Wave Systems, Inc., for computing a certain type of Boolean tensor decomposition called Boolean Hierarchical Tucker Network (BHTN). Boolean tensor decomposition problems ask for finding a decomposition of a high-dimensional tensor with categorical, [true, false], values, as a product of smaller Boolean core tensors. As the BHTN decompositions are usually not exact, we aim to approximate an input high-dimensional tensor by a product of lower-dimensional tensors such that the difference between both is minimized in some norm. We show that BHTN can be calculated as a sequence of optimization problems suitable for the D-Wave 2000Q quantum annealer. Although current technology is still fairly restricted in the problems they can address, we show that a complex problem such as BHTN can be solved efficiently and accurately.

Sensitivity Operator-Based Approach to Heterogeneous Air Quality Monitoring Data Analysis

A. Penenko, V. Penenko, E. Tsvetova, A. Gochakov, E. Pyanova, V. Konopleva

The joint use of atmospheric chemistry transport and transformation models and observational data makes it possible to solve a wide range of environmental-protection tasks, including pollution sources identification and reconstruction of the pollution fields in unobserved areas. Air quality monitoring systems vary in their temporal and spatial coverage, the composition of the observed chemicals, and the accuracy of measurements. Seamless utilization of different data types can improve the accuracy of air quality analysis and forecast systems. The approach considered is based on sensitivity operators and adjoint equations solutions ensembles. The source identification problem for the advection-diffusion-reaction model is transformed into a quasi-linear operator equation with a sensitivity operator. The sensitivity operator is constructed of the sensitivity functions' ensemble, corresponding to the measurement data elements. This ensemble construction allows for the natural combination of various measurement data types in a single operator equation. In the paper, we consider a combined use of image-type, integral-type, *in situ*, and time-series-type measurement data for the air pollution source identification problem. The approach is illustrated in a numerical experiment.

Synergy between Convergence and Divergence Review of Concepts and Methods

K. Penev

Modern Industry 4.0 technologies face a challenge in dealing with billions of connected devices, petabyte-scale of generated data, and exponentially growing internet traffic. Artificial Intelligence and Evolutionary algorithms can resolve variety of large optimisation problems. Many methods employed in search for solutions often fall in stagnation or in unacceptable results, which reminds for classical dilemma exploration versus exploitations closely related with convergence and diversity of the explored solutions. This article reviews convergence and divergence centred algorithms and discuses synergy between convergence and divergence in adaptive heuristics.

Convergence of the Value Function in Optimal Control Problems with Uncertain Dynamics

A. Pesare, M. Palladino, M. Falcone

We deal with the convergence of the value function of an approximate control problem with uncertain dynamics to the value function of a nonlinear optimal control problem. The assumptions on the dynamics and the costs are rather general and we assume to represent uncertainty in the dynamics by a probability distribution. The proposed framework aims to describe and motivate some model-based Reinforcement Learning algorithms where the model is probabilistic. We also show some numerical experiments which confirm the theoretical results.

Computational Study of IL-6 Inhibition by Low-Molecular-Weight Heparin

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

Interleukine 6 (IL-6) is a pleiotropic cytokine with an important role in inflammation, immune response, and hematopoiesis. The intracellular signalling is initiated after a two-stage process of formation of the triple complex of IL-6, IL-6 receptor (IL-6Rα) and a second membrane protein, glycoprotein 130 (gp130), and its subsequent dimerisation. Aberrant IL-6 levels are associated with chronic inflammation and autoimmunity. In addition, the cytokine has been recognized as a key participant in the development of an acute severe systemic inflammatory response – the acute cytokine release syndrom (CRS), known also as cytokine storm (CS). Therefore, searching for an inhibitor of the IL-6 signalling cascade is of interest for the management and treatment of CS. One possible

candidate, able to bind to IL-6 is low-molecular-weight heparin (LMWH). LMWH are highly sulfated polysaccharide chains with a very high electric-charge density, determining their very high biological activity.
Here, we report the results of a computational study of the interaction of LMWH hexasaccharides with IL-6 and the macromolecular complexes IL-6/IL-6Rα and IL-6/IL-6Rα/gp130. We show that heparin forms a stable complex with IL-6, blocking one of its binding sites and thus inhibiting the formation of the IL-6/IL-6R complex. In addition, LMWH molecules also bind to the IL-6/IL-6Rα complex, blocking another binding site in IL-6, and thus preventing proper recruitment of the gp130 receptor. Our results reveal the mechanism of heparin inhibitory action on the IL-6 activity.

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Quality Optimization of Seismic-Derived Surface Meshes of Geological Bodies

P. Popov, V. Iliev, G. Fitnev

Availability of 3D datasets of geological formations present a number of opportunities for various numerical simulations provided quality meshes can be extracted for the features of interest. We present a particular technique designed to generate an initial levelset-based triangulation of geological formations such as salt volumes, turbidites, faults and certain types of shallow horizons. We then work directly with the underlying voxel data to improve the mesh quality so that the resulting triangulation is suitable for numerical simulations involving PDEs, while approximating well enough the underlying (implicit) levelset. We apply our algorithm on typical Gulf of Mexico formations including turbidite reservoirs and multiple salt domes. We demonstrate that the resulting meshes are of high quality and can be directly used in coupled poroelastic reservoir simulations.

First Order Reaction-Diffusion System with Riesz-Type Space-Fractional Diffusion

D. Prodanov

Diffusion in porous media, such as biological tissues, is characterized by deviations from the usual Fick's diffusion laws, which can lead to space-fractional diffusion. The Riesz

operator can be easily understood in the Fourier domain where $(-\Delta)^q \mapsto |k|^{2q}$. The present contribution considers the system

$$\partial_t c = -D(-\Delta)^q c + s - \kappa c, \quad 0 < q \leq 1$$

where s is a constant spatially-extended source, D is the diffusion constant, κ is an elimination constant, and c is the concentration of the diffusing species. The problem arises in the modelling of controlled release of substances and biomedical engineering [1]. I consider the simple case of two spatial compartments – a proximal one of finite width having a source; and a distal one, which is extends to infinity and the source is not present. The present contribution considers cylindrical geometry, where the steady state concentration c_s can be represented as a Hankel transform:

$$c_s(r) = s \int_0^\infty \frac{J_0(r\rho)\rho}{\rho^{2q} + \kappa} d\rho$$

in the distal compartment. The presentation considers the computation of the integral using the double-exponential quadrature integration technique [2], compared to the Maixma integration routine QUADPACK [3].

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Efficient Solvers for Poromechanics

F. A. Radu

In this talk we present efficient numerical schemes for linear and nonlinear Biot models [1,2]. Nonlinear Lame coefficients and/or fluid compressibility or large deformations are considered. Furthermore, an erosion problem with a moving boundary is presented [3]. We use the L-scheme, see e.g. [4] or the Newton method for linearization, either monolithically or combined with a fixed stress type splitting [5,6]. Additionally, the optimisation of the stabilisation parameter in the fixed-stress scheme will be discussed [7].

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Exact and Efficient Structured Tensor Decomposition

E. Robeva

In this talk we will discuss several types of structured tensor decompositions which can be done efficiently. First, we will discuss orthogonally decomposable tensors. Extending this notion, we will see that one can decompose exactly and efficiently certain frame decomposable tensors. Finally, we will discuss how to decompose tensor trains which have orthogonally decomposable tensors at their nodes.

Neural Networks Applied to a Morphoelastic Model for Skin Contraction

M. Schaaphok, G. Egberts, F. Vermolen

Deep tissue injury is often characterised by contraction of skin tissue. In extreme cases, this contraction can give the side-effect that the patient becomes immobile. In such pathological situations, one speaks of a contracture. In order to be able to predict and to improve treatments in a way that no, or just little animal testing is needed, mathematical models are an interesting tool. To incorporate permanent deformations as a result of large displacements and changes of the microstructure of tissue, we use a morpho-elastic model. This model was firstly developed by Rodrigues, and further extended by Gorieli, as far as we know. The model involves a nonlinearly coupled set of equations, where a finite element method is used to approximate the solution. During the talk, we will present some of our stability analysis.
Many of the input variables in our model are patient-specific, which is an important source of uncertainty in the simulations. This is the reason why we merely aim at predicting the likelihood that a scenario occurs rather than predicting the scenario itself. Since this step requires many sample computations that are expensive, we study the possibility to use artificial intelligence to mimic the finite element results. The idea is to provide the clinicians with a trained neural network-based model of the problem. These simulations can be obtained within very short calculation times. Furthermore, the trained neural network should be enriched with clinical observations in the future.

Reduced Basis Methods for Efficient Simulation of a Rigid Robot Hand Interacting with Soft Tissue

S. Shuva, O. Röhrle, B. Haasdonk

In this contribution, we present efficient reduced basis methods for the simulation of the coupled problem consisting of a rigid robot hand interacting with soft tissue material. To model the problem, we use the time-dependent linear elasticity partial differential equation (PDE) from continuum mechanics. The problem is formulated in two ways: (i) forward simulation of the coupled problem, where the robot hand along with the soft tissue material follows a prescribed trajectory, and (ii) a feedback controller is designed in such a way that the robot hand along with the soft tissue material cost-optimally reaches a target position and then stabilizes. We apply the finite element method to tackle the problems numerically. As a result in both cases, large dimensional systems of equations appear, which need to be solved in real-time. This is very essential in practice for the implementation of the above mentioned scenarios in a real robot. For the second case, in the context of the linear quadratic regulator (LQR), we encounter a large-scale Algebraic Riccati Equation (ARE). To overcome the real-time contraint by significantly reducing the computational complexity, we use several structure-preserving and non-structure-preserving reduction methods. These include proper orthogonal decomposition (POD) -based reduced basis techniques. For the ARE, instead of solving a full dimensional problem we compute a low-rank-factor and hence a low-dimensional ARE is solved. Numerical examples for both cases are provided. These illustrate the approximation quality of the reduced solution and speedup factors.

Hierarchical Compression Solver for Parabolic Problems with Space-Fractional Diffusion

D. Slavchev, S. Margenov

Equations involving fractional diffusion operators are used to model anomalous processes in which the Brownian motion hypotheses are violated.
We consider the parabolic problem

$$\frac{\partial u(x,t)}{\partial t} + L^\alpha u(x,t) = f(x,t), \quad \alpha \in (0,1),$$

where L^α stands for the integral fractional Laplacian defined trough the Ritz potential, and homogeneous Dirichlet boundary conditions are assumed. Linear finite elements are used for discretization in space, thus obtaining the Cauchy problem

$$M_L \frac{d\mathbf{u}}{dt} + A\mathbf{u} = M_L\mathbf{f}, \quad 0 < t \leq T, \quad \mathbf{u}(0) = \mathbf{u^0},$$

where A is the matrix corresponding to the approximation of L^α and M_L is the lumped mass matrix. The backward Euler scheme

$$M_L \frac{\mathbf{u}^{j+1} - \mathbf{u}^j}{\tau_j} + A\mathbf{u}^{j+1} = M_L\mathbf{f}^j, \quad j = 1, \ldots, m,$$

is used for discretization in time, where $\sum_{j=1}^{m} \tau_j = T$. Therefore, at each time step j we solve a linear system with the matrix $\frac{1}{\tau_j} M_L + A$.
Let us recall that the fractional diffusion matrix A is dense. Hierarchical compression is applied to improve the computational efficiency of the time stepping algorithm. The STRUMPACK (STRUctured Matrices PACKage) software package is utilized in the developed parallel solver. We presented scalability analysis varying the number of processors (cores) and the size of discretization parameters in space and time.

Acknowledgements
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Using the Cauchy Criterion and the Standard Deviation to Evaluate the Sustainability of Climate Simulations

V. Spiridonov, H. Chervenkov

In simulations of climate change with climate models, the question arises as to whether the accepted 30-year period is sufficient for the model to produce sustainable results. We are looking for an answer to this question using the Cauchy criterion and the idea of saturation suggested by Lorenz, using as a sufficient condition for saturation the requirement that the standard deviation should not increase from year to year.
The proposed method is illustrated by analysis of time series of real observations of the temperature at 2 m and of three global climate models for the same parameter. The measured data are for the Cherni Vrah peak of Vitosha Mountain in Bulgaria and the modelled data, which concerns the projected future climate up to year 2100, are taken from the Climate Data Store of the Copernicus project. The example of the real observations shows the instability of meteorological processes since 2000 year. All three global climate models, forced with the CMIP5 RCP4.5 scenario, show a lack of sustainability in the polar regions for the period 2071–2100.

Nonnegative Matrix and Tensor Factorizations in the Analysis of Scientific Text Documents

V. Stanev, B. Aleksandrov

The dramatic growth of the volume of scientific publications presents a huge challenge to individual researchers and research organizations, making it virtually impossible to keep up with the relevant literature. This creates a large demand for advanced AI methods that can be used to organize text documents and to summarize their content in a human-friendly format. In this context particularly important are various tools for topic modeling. One of the primary objectives of text mining, topic modeling has been used extensively to automate the analysis of large text corpora. In this talk I will present recent research utilizing Nonnegative Matrix Factorization (NMF) and Nonnegative Tensor Factorization (NTF) methods for topic modeling of scientific abstracts. I will present an analysis of a corpus consisting of a large number of abstracts of physics papers. Using NMF and NTF, we were able to detect the latent topics in the corpus, as well as the topic evolution and the communities of authors contributing to each

topic. The use of NMF and NTF allowed us to incorporate a robust system for determining the optimal number of latent topics, which is crucial for the retrieval of meaningful topics. Thus, these methods are a promising avenue for scientific corpora analysis.

Large-Scale Computer Simulation of the Performance of the Generalized Nets Model of the LPF-algorithm

T. D. Tashev, A. K. Alexandrov, D. D. Arnaudov, R. P. Tasheva

A crossbar switch node maximizes the speed of data transfer using parallel existing paths between the input and output lines of the switch node. For this purpose computation of a non-conflict schedule is performed by the control block of the node. The computational problem is NP-complete. The problem of developing more effective algorithms for non-conflict scheduling is attracting much attention in the current literature.
Previously we have developed a non-conflict scheduling MiMa-algorithm (Minimum of Maxima algorithm). In this paper, we present large scale simulations for comparison of the throughput of our MiMa-algorithm with the throughput of an existing LPF-algorithm (Longest Port First algorithm). Both algorithms are of the same type ("weight" type), but the MiMa-algorithm is deterministic while the LPF-algorithm employs a Monte Carlo method.
The presented simulations are performed for large sizes of the switch field (for $n \in [2, 101]$) and are executed on the supercomputer AVITOHOL located at the IICT-BAS. The throughput for Generalized Nets (GN) models of both algorithms are studied for i.i.d. Bernoulli uniform load traffic.
Problems arose due to the time complexity of the implementation of the LPF-algorithm (O(n $^{4.7}$)). It was necessary to reduce the time complexity without introducing distortions into the results of simulation. The variant of the LPF-algorithm with simplified random selection of the initial element of the traffic-matrix was proposed. Its complexity has been reduced over time to (O (n $^{3.8}$)). This made it possible to meet the resource constraints in time when using the AVITOHOL supercomputer.
The results of our study show that the LPF-algorithm has a slight advantage (about 3 %) with respect to the throughput while the MiMa-algorithm is advantageous with respect to the execution time. We have discussed possibilities for improving the performance of the MiMa-algorithm.

Advanced Stochastic Aproaches Based on Optimization of Lattice Sequences for Large-Scale Finance Problems

V. Todorov, I. Dimov, R. Georgieva, S. Apostolov, S. Poryazov

Computational finance is one of the most important topic nowadays. Nowadays Monte Carlo (MC) and quasi-MonteCarlo (QMC) methods have become a popular computational device for problems in finance. The field of mathematical finance is becoming more sophisticated and quantitative andthe scope of its applications is growing. The QMC methods using special deterministic sequences achieve higher accuracy and computational efficiency compared to the

MC methods. Options have been widely tradedsince the creation of the organized exchange in 1973. The famous Black-Scholes model provides explicit closed form solutions for the values of the European style call and put options.
Different optimal generating vectors have been applied for the first time to a specific problem in computational finance and they give superior results to the stochastic approaches used up to now. Since the performance of the lattice rule depends on the choice of the generator vectors,the optimal vectors is an optimization over the Fibonacci generalized vector and other generating vectors used up to now.
The main advantage of the developed algorithms is their linear computational complexity with respect to dimension, while the deterministic methods suffer from the so-called curse of dimensionality and they become impractical in higher dimensions. The best performance of the optimization method is explained by the choice of the optimal generating vectors, whose computation uses fast component-by-component operations.
Clearly, the progress on the problem of option pricing and other problems in the computational finance area is closely related to the development of reliable algorithms for multidimensional numerical integration.

Multidimensional Sensivitity Analysis for AIr Pollution Model Based on Modifications of the Van der Corput Sequence

V. Todorov, T. Ostromsky, I. Dimov, R. Georgieva, Z. Zlatev

The present study is based on The Unified Danish Eulerian Model (UNI-DEM) as one of the most advanced large-scale mathematical models that describes adequately all physical and chemical processes. One of the most attractive features of UNI-DEM is its advanced chemical scheme the Condensed CBM IV, which consider a large number of chemical species and numerous reactions between them, of which the ozone is one of the most important pollutants for its central role in many practical applications of the results. The calculations are done in a large spatial domain, which covers completely the European region and the Mediterranean, for certain time period.
Variance-based methods are most often used for providing sensitivity analysis. Two of the most commonly used variance-based methods were applied in our study: *Sobol approach* and *Fourier Amplitude Sensitivity Test (FAST)*. These were implemented by using Monte Carlo algorithms. Quasi-Monte Carlo algorithms are based on quasirandom or low discrepancy sequences which are "less random" than a pseudorandom number sequence, but more useful for numerical computation of integrals in higher dimensions, because low discrepancy sequences tend to sample space "more uniformly" than random numbers.
Some modifications of the Van der Corput sequence are studied in our numerical experiments. The modifications of the Van der Corput sequence is often used to generate a "subrandom" sequence of points which have a better covering property than pseudorandom points.
A comprehensive experimental study of highly efficient stochastic approaches based on the Van der Corput sequence and its modification with specific choice of the bases for multidimensional integration has been done for the first time for the particular model.

Intuitionistic Fuzzy Approach for Outsourcing Provider Selection in a Refinery

V. Traneva, S. Tranev

Outsourcing is the transfer of a business process that has been traditionally operated and managed internally to an independently owned external service provider. Outsourcing is a good strategy for firms that need to reduce operating costs and improve competitiveness and it is important that firms select out the most eligible outsourcing providers.
In this study, an intuitionistic-fuzzy multi-criteria decision making approach for choosing the most eligible outsourcing service provider for an oil refining enterprise on the Balkan peninsula which has decided to outsource some maintenance activities in order to make its core business more efficient and more competitive. The optimal autsoursing problem is formulated and an algorithm for selection the most eligible outsourcing service provider is proposed using the consept of index matrices (IMs), where the evaluations of outsourcing candidates against criteria formulated by several experts are intuitionistic fuzzy pairs. The proposed decision model takes into account the ratings of the experts and the weighting factors of the evaluation criteria according to their priorities for the outsourcing service. Due to the complexity of outsourcing process, the real numbers are not enough to characterize the evaluation objects. Fuzzy sets (FSs) of Zadeh use the single membership function to express the degree to which the element belongs to the fuzzy set. As a result, the FSs is unable to express the non-membership degree and hesitation degree. Since intuitionistic fuzzy sets (IFSs) of Atanassov consider the membership and non-membership degrees simultaneously, it is more flexible than the FSs in dealing with uncertainty.
The originality of the paper comes from the proposed decision model and application of the model in the outsourcing problem of a refinery. The presented approach for selection the most appropriate outsourcing service provider can be applied to problems with imprecise parameters and can be extended in order to obtain the optimal solution for other types of multidimensional outsoursing problems by using n-dimensional index matrices.

Neural Network-based Model Order Reduction for solving parametrized nonlinear reaction-diffusion systems

K. Urban, M. Youssef

The Reduced Basis Method (RBM) is a very well-established model order reduction technique for parametrized partial differential equations (PPDEs). The RBM consists of an offline training stage to create the reduced model (a linear space) and an online stage to determine a reduced solution highly efficient in terms of a Galerkin projection onto the reduced space. However, the limitation of such a linear approximation is known, the RBM shows poor convergence rates e.g. for transport or wave-type equations. Thus, nonlinear model reduction techniques are needed.
We present a novel *nonlinear* model reduction approach using neural networks. In the offline stage, we use a greedy algorithm to train neural networks both for the the quantity of interest (QoI) of the PPDE as well as for the corresponding error (bound). In the online stage, we simply evaluate these previously trained neural networks to obtain an approximation for the QoI as well as an error bound for given new values of the parameters.

We illustrate the quantitative performance of the derived model-order reduction by parameterized nonlinear reaction-diffusion systems

$$\begin{aligned} \frac{\partial T(x,t)}{\partial t} &= \nabla^2 T(x,t) + a\ (C(x,t)+1)\ \mathrm{e}^{-\gamma/(T(x,t)+1)} \\ \frac{\partial C(x,t)}{\partial t} &= b\,\nabla^2 C(x,t) - d\ (C(x,t)+1)\ \mathrm{e}^{-\gamma/(T(x,t)+1)}, \end{aligned} \tag{1}$$

with initial conditions

$$T(x,0) = 0, \qquad C(x,0) = \frac{1}{(3x+1)^2} - 1, \tag{2}$$

and boundary conditions

$$T(0,t) = 0 = T(1,t), \qquad C(0,t) = 0 = \frac{\partial C}{\partial x}|_{x=1} \tag{3}$$

Decoupling Methods for Systems of Parabolic Equations

P. N. Vabishchevich

We consider the decoupling methods of the Cauchy problem's numerical solution for a system of multidimensional parabolic equations. Of most significant interest for computational practice is the case when the equations are related to each other. Splitting schemes are constructed for such vector problems when the transition to a new layer in time is provided by solving common scalar problems for individual components of the solution.
Two main classes of decoupling methods are distinguished by allocating the diagonal part of the problem's matrix operator and its lower and upper triangular parts. An increase in the approximate solution of explicit-implicit schemes is achieved by using some three-layer approximations in time. Special attention is paid to when the time derivatives of the solution components are related to each other.

Numerical Solution of Non-Stationary Problems with a Rational Approximation for Fractional Powers of the Operator

P. N. Vabishchevich

The numerical solution of the Cauchy problems for a first and second-order differential-operator equation are discussed. A fundamental feature of the problem under study is that the equation includes a fractional power of the self-adjoint positive operator. In computational practice, rational approximations of the fractional power operator are widely used in various versions. We construct special approximations in time when the transition to a new level in the time provided a set of standard problems for the operator and not for the fractional power operator. Stable splitting schemes with weights parameters are proposed for the additive representation of rational approximation for a fractional power operator.

On the Interplay Between Coarsening in AMG and Data Clustering in Graphs

P. S. Vassilevski

We consider a popular community detection algorithm for data represented by undirected graphs and relate it to the coarsening by aggregation in AMG (algebraic multigrid). In particular, we bring together two popular algorithms: one is the Luby's parallel matching algorithm used to create AMG aggregates, whereas the weights assigned to the graph edges are based on the graph modularity functional that is being very successfully used in community detection. As an application, we propose a new version of the so-called adaptive AMG that improves its convergence after each step of adaptation. On the other hand, the near-null component vectors computed by the adaptive AMG provide vertex coordinates for graph embedding in R^d that can be used in the popular K-means algorithm as well as in graph visualization (for $d = 2$ or 3).

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Numerical Schemes for Simulation of Incompressible Flows in Time-Dependent Domains

Y. Vassilevski, M. Olshanskii, A. Lozovskiy, A. Danilov

We present stable finite-element schemes for simulation of incompressible flows in time-dependent domains. The time step is independent of the mesh size, and only one linear system is solved on each time step. We consider fluid-structure interaction (FSI) and Navier-Stokes equations in time-dependent domains. The properties of the scheme are shown on several benchmarks and hemodynamic applications.
In particular, we address 2D and 3D flows in blood vessels with nonlinear hyperelastic models of vessel wall, steady and periodic interactions between a viscous incompressible fluid and a nonlinear solid filament in a 3D setting for which experimental data are collected using phase-contrast magnetic resonance imaging. We also present simulation of an incompressible flow in a model of the left ventricle of the human heart, where the ventricle wall dynamics is reconstructed from a sequence of contrast enhanced Computed Tomography images.

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Structured Deep Kernel Networks for Data-Driven Modeling of Turbulent Flows

T. Wenzel, G. Santin, M. Kurz, A. Beck, B. Haasdonk

Standard kernel methods for machine learning usually struggle when dealing with high-dimensional and large data sets. Based on a Representer Theorem for Deep Kernel learning, we propose a Structured Deep Kernel Network that is capable of dealing with high-dimensional and huge data sets - thus alleviating two major drawbacks of standard methods. We show approximation results for these Structured Deep Kernel Networks, which confirm their use for machine learning applications.
We apply the proposed setup to the numerical simulation of turbulent flows, in particular to the data-driven prediction of closure relations. A main challenge of this application is given by the high dimensionality of the large data sets, which the proposed Structured Deep Kernel Network is able to deal with. This surrogate modeling thus provides a significant acceleration of the overall turbulence simulation. A comparison with Neural Network approaches is provided and highlights the benefits of Structured Deep Kernel Networks.

A Posteriori Error Estimates for Biot Systems Using Fixed-Stress Splitting

M. F. Wheeler, X. Lu, V. Girault

We analyze the Biot system solved with a fixed-stress split, Enriched Galerkin (EG) or Galerkin discretizations for the flow equation, and Galerkin for the mechanics equation. Residual-based a posteriori error estimates are established with both lower and upper bounds. These theoretical results are confirmed by numerical experiments performed with Mandels problem. The efficiency of these a posteriori error estimators to guide dynamic mesh refinement is demonstrated We further propose a novel stopping criterion for the fixed-stress iterations using the error indicators to balance the fixed-stress split error with the discretization errors. The new stopping criterion does not require hyperparameter tuning and demonstrates efficiency and accuracy in numerical experiments.

Locking Free and Locally Conservative Enriched Galerkin Methods for Poroelasticity

S.-Y. Yi, S. Lee, L. Zikatanov

We present a novel enriched Galerkin (EG) finite element discretization for the numerical modeling of a poroelastic system. A new locking free EG method is proposed for the mechanics problem, and a locally conservative EG method is used to discretize the flow problem. These methods utilize the well-known interior penalty discontinuous Galerkin (DG) techniques, but the approximation spaces have much less degrees of freedom than typical DG spaces, thus offering

an efficient alternative to DG methods for numerical models in poromechanics. Furthermore, we show a priori error estimates of optimal order in the energy norm, independent of the Lame parameters. As a result, the proposed method is free of volumetric locking when modeling incompressible materials. We also introduce a preconditioner for EG, uniform with respect to the mesh size in the operator preconditioning framework. Several numerical examples confirm the accuracy and the robustness of the EG discretizations and the preconditioner.

Domain Decomposition and Partitioning Methods for Mixed Finite Element Discretizations of the Biot System of Poroelasticity

I. Yotov

We develop non-overlapping domain decomposition methods for the Biot system of poroelasticity in a mixed form. The solid deformation is modeled with a mixed three-field formulation with weak stress symmetry. The fluid flow is modeled with a mixed Darcy formulation. We introduce displacement and pressure Lagrange multipliers on the subdomain interfaces to impose weakly continuity of normal stress and normal velocity, respectively. The global problem is reduced to an interface problem for the Lagrange multipliers, which is solved by a Krylov space iterative method. We study both monolithic and split methods. In the monolithic method, a coupled displacement-pressure interface problem is solved, with each iteration requiring the solution of local Biot problems. We show that the resulting interface operator is positive definite and analyze the convergence of the iteration. We further study drained split and fixed stress Biot splittings, in which case we solve separate interface problems requiring elasticity and Darcy solves. We analyze the stability of the split formulations. Numerical experiments are presented to illustrate the convergence of the domain decomposition methods and compare their accuracy and efficiency.
This is joint work with Manu Jayadharan and Eldar Khattatov.

Reinforcement Learning with Guarantees

M. Zanon, S. Gros

Reinforcement Learning (RL) is a data-driven technique which aims at solving Markov Decision Processes (MDPs) by relying on samples of the observed instantaneous cost. This approach allows one to solve MDPs without the need to know the model of the Markov Chain (MC). However, in the same way as Dynamic Programming (DP), RL is also affected by the curse of dimensionality. In order to circumvent this issue, the solution is often approximated by a parametric function, e.g., a neural network. This approach allows one to reduce the dimension of the search space and, therefore be able to compute an approximate solution. Recent progress has obtained stunning achievements, such as learning to fly a helicopter or how to walk without prior knowledge.
The main issue with RL and MDPs in general, is the difficulty in guaranteeing desirable properties such as stability and safety (in the sense of constraint satisfaction). Moreover, in model-free

methods, it is hard to obtain some form of explainability of what the closed-loop system will do in the future. Model-based methods, instead, allow one to predict the future system behavior and, therefore, be able to obtain some insight in the problem. In our recent work, we have proposed a new function approximator based on Model Predictive Control (MPC): a model-based finite-horizon discrete-time optimal control problem, which can directly support the policy, the value function and the action-value function. These functions are defined implicitly, since one needs to solve MPC in order to evaluate them. We propose to parametrize them by parametrizing the cost and constraints defining the MPC scheme and let RL adapt the parameter so as to solve the MDP. The first result we proved is that, even though the model in MPC does not exactly match the MC, it is still possible to recover the exact MDP solution. Then, we proved that one can restrict the MPC stage cost to be positive-definite, provided that an initial cost is also learned. This is a desirable property both for numerical solvers in MPC and for proving stability. Finally, we have proven that, provided that the problem is suitably formulated, both constraint satisfaction and asymptotic stability can be enforced, by introducing simple constraints on the parameter.

Quantitative Relationship Between High Concentrations of Particulate Matter and Morbidity in Sofia

P. Zhivkov, A. Simidchiev

Air pollution is a major environmental health problem affecting everyone. According to the World Health Organization (WHO), there is a close relationship between small particles (PM10 and PM2.5) and increased morbidity or mortality, both daily and over time. We investigated this quantitative relationship in Sofia by comparing levels of particulate matter with a baseline number of hospital, emergency department visits, asthma prevalence, and other morbidity outcomes from 4 local health sources. The methods for this comparison model are linear correlation and non-parametric correlation analysis of a time series study conducted in Sofia from 1 January 2017 to 31 May 2019. We introduce in this study an optimized spatial and time coverage of air quality by including data from a network of citizen stations. These benefits are weighed against limitations, such as model performance, the precision of the data in days with high humidity, and the appropriateness of which will depend on epidemiological study design. The final results that will be presented can be used for optimizing healthcare and pharmaceutical planning by justifying what acute morbidities are mostly affected by higher concentrations of PM10 and PM2.5.

Running an Atmospheric Chemistry Scheme from a Large Air Pollution Model by Using Advanced Versions of the Richardson Extrapolation

Z. Zlatev, I. Dimov, I. Faragó, K. Georgiev, Á. Havasi

Atmospheric chemistry schemes, which are described mathematically by non-linear systems of ordinary differential equations (ODEs), are used in many large-scale air pollution models.

These systems of ODEs are badly-scaled, extremely stiff and some components of their solution vectors vary quickly forming very sharp gradients. Therefore, it is necessary to handle the atmospheric chemical schemes by applying accurate numerical methods combined with reliable error estimators. Three well-known numerical methods that are suitable for the treatment of stiff systems of ODEs were selected and used: (a) EULERB (the classical Backward Differentiation Formula), (b) DIRK23 (a two-stage third order Diagonally Implicit Runge-Kutta Method and (c) FIRK35 (a three-stage fifth order Fully Implicit Runge-Kutta Method). Each of these three numerical methods was applied in a combination with nine advanced versions of the Richardson Extrapolation in order to get more accurate results when that is necessary and to evaluate in a reliable way the error made at the end of each step of the computations. The code is trying at every step (A) to determine a good stepsize and (B) to apply it with a suitable version of the Richardson Extrapolation so that the error made at the end of the step will be less than an error-tolerance TOL, which is prescribed by the user in advance. The numerical experiments indicate that both the numerical stability can be preserved and sufficiently accurate results can be obtained when each of the three underlying numerical methods is correctly combined with the advanced versions of the Richardson Extrapolation.

Part C

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