KLAIM 2023

Kaiserslautern Applied and Industrial Mathematics Days

KLAIM 2023, September 25 to 27, 2023
Book of Abstracts

Synthesis of Models and Data

KLAIM 2023 is jointly hostet by Fraunhofer Institute for Industrial Mathematics ITWM and the Department of Mathematics of the University of Kaiserslautern-Landau (RPTU).

KLAIM 2023
Kaiserslautern Applied and Industrial Mathematics Days

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Welcome to KLAIM 2023: Synthesis of Models and Data

September 2023

Dear Participants,

A cordial welcome to all of you! We are looking forward to the second edition of the Kaiserslautern Applied and Industrial Mathematics Days – KLAIM 2023 with hopefully many opportunities for scientific exchange and lively discussions.

The purpose of this workshop is to provide a forum for applied mathematicians from academia, research labs and industry in order to discuss recent results and to move forward into new research fields. After the successful start of this conference series in 2021 where Digital Twins stood for the conference motto, we continue this year by putting emphasis on the Synthesis of Models and Data. This thematic focus addresses in particular the combination of model-based approaches and data-driven techniques, leading thus to hybrid learning frameworks.

The workshop is hosted jointly by the Fraunhofer Institute for Industrial Mathematics ITWM and the Department of Mathematics at the University of Kaiserslautern-Landau (RPTU). The program will be structured along the following five tracks:

1. Models and Data across Scales and Domains in Engineering Applications
2. Risk Management and Machine Learning
3. Simulation and Optimization in Fluid Dynamics
4. Mathematical Programming: Uncertain Data and Multiple Objectives
5. Analyzing Materials Structures: Images, Machine Learning and Stochastic Geometry

Additionally, we have organized a special session on **“Mathematical Research Data”**.

Mathematics in Kaiserslautern

Applied and industrial mathematics with its two study programs Economathematics and Technomathematics has a long and remarkable tradition in Kaiserslautern, dating back to 1979. Today, the department of Mathematics at the RPTU has been evaluated to be in the top group of all German mathematics departments in the latest university rankings. It has a high reputation for its research profile and for its international programs at the master and PhD levels. The Fraunhofer ITWM is one of the leading institutes in industrial mathematics worldwide, and from its beginning there has been a strong cooperation between the RPTU and the Fraunhofer ITWM.

The Fraunhofer ITWM, which was founded in 1996, has successfully completed more than 2500 projects in cooperation with industry in the past ten years. Nearly 550 people are currently working at Fraunhofer ITWM, including 60 PhD students and 150 undergraduate students. The mathematics location Kaiserslautern is excellently networked in the scientific community through joint projects and presentations at international congresses and conferences. The scientists from Kaiserslautern have contributed significantly to the development of the European Consortium for Mathematics in Industry (ECMI).

Dankeschön!

We gratefully acknowledge the support from MathAPP – Mathematics applied to real-world problems, which is is part of the Rhineland-Palatinate research initiative and sees itself as an interdisciplinary potential area that promotes the networking of mathematics and engineering sciences and the associated scientists.

Finally, a special and warm "Dankeschön" goes to those people who work behind the scenes to make KLAIM 2023 a success: Stephanie Beck, Gesa Ermel, Steffen Grützner, Doris Hemmer-Kolb, and Esther Packullat.

Anita Schöbel

Bernd Simeon

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KLAIM 2023
Kaiserslautern Applied and Industrial Mathematics Days

Preliminary Program

Monday, September 25, 2023

	Auditorium	Seminar room Z03.07/08
13:30	**Welcome** Sven O. Krumke (RPTU), Anita Schöbel (Fraunhofer ITWM), Bernd Simeon (RPTU)	
13:40	**Plenary A.59 Reliable AI: Successes, Challenges, and Limitations**[1] Gitta Kutyniok, Ludwig-Maximilians-Universität (LMU), Munich, DE	
14:30	**ANALYZING MATERIALS STRUCTURES: IMAGES, MACHINE LEARNING AND STOCHASTIC GEOMETRY**	**MODELS AND DATA ACROSS SCALES AND DOMAINS IN ENGINEERING APPLICATIONS**
	A.54 Random Tessellation Forests for High-dimensional Data (Track Plenary)[1] Eliza O'Reilly, Johns Hopkins University, US	**A.30 Dynamic Human Body Models in Vehicle Safety: An Overview (Track Plenary)**[1] Jörg Fehr, University of Stuttgart, DE
	A.04 Large-scale statistical learning for mass transport prediction in porous materials using 90,000 artificially generated microstructures[2] Benedikt Prifling, Ulm University, DE	**A.15 Concurrent two-scale simulations in solid mechanics with Deep Material Networks**[2] Matti Schneider, Karlsruhe Institute of Technology (KIT), DE
	A.53 A variational perspective on auxetic metamaterials of checkerboard-type[2] Dominik Engl, Catholic University of Eichstätt-Ingolstadt (KU), DE	**A.01 From Disruption to Success: Predictive Analytics in presence of Structural Changes in Energy systems**[2] Milena Petkovic, Zuse Institute Berlin, DE
16:00	Coffee break	
16:30	**MATHEMATICAL PROGRAMMING: UNCERTAIN DATA AND MULTIPLE OBJECTIVES**	**RISK MANAGEMENT AND MACHINE LEARNING**
	A.57 Recent Advances in Discrete and Robust Bilevel Optimization (Track Plenary)[1] Ivana Ljubic, ESSEC Business School, Paris, FR	**A.55 A stochastic gradient descent algorithm to maximize power utility of large credit portfolios under Marshall-Olkin dependence (Track Plenary)**[1] Matthias Scherer, Technical University of Munich, DE
	A.10 A 3-stage adaptive algorithm for nonlinear robust optimization[2] Kerstin Schneider, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE	**A.18 Active Learning of Surrogate Models for Inverse Problems**[2] Martin Weiser, Zuse Institute Berlin, DE
	A.43 Adjustable Robust Optimization for Transport Planning with Uncertain Demands[2] Sabina Kiss, s2 data & algorithms, Graz, AT	**A.22 A certified adaptive surrogate hierarchy for parametrised reactive flow**[2] Felix Schindler, Mathematics Münster, DE
18:00	End of conference day 1	

Tuesday, September 26, 2023

	Auditorium	Seminar room Z03.07/08
9:00	**Plenary A.60 Model Order Reduction at Industrial Scale**[1] Peter Benner, Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, DE	
9:50	**MATHEMATICAL PROGRAMMING: UNCERTAIN DATA AND MULTIPLE OBJECTIVES**	**RISK MANAGEMENT AND MACHINE LEARNING**
	A.32 Applying Reverse Search Enumeration to Tri-Objective Linear Programming: A New Way to Parallelize Finding Extreme Points[2] Levin Nemesch, University of Kaiserslautern-Landau, DE	**A.40 Scenario generation for market risk models using generative neural networks**[2] Solveig Flaig, Deutsche Rückversicherung AG, Düsseldorf, DE
	A.39 The Weighted p-Norm Weight Set Decomposition for Multiobjective Discrete Optimization Problems[2] Kathrin Prinz, University of Kaiserslautern-Landau, DE	**A.41 Calculating Expectiles and Range Value-at-Risk using Quantum Computers**[2] Christian Laudagé, University of Kaiserslautern-Landau, DE
	A.37 Finite representation of quantile sets for multivariate data via vector linear programming[2] Andreas Löhne, Friedrich-Schiller-Universität, Jena, DE	**A.45 Risk Management in Portfolio Optimization: A Multicriteria Approach**[2] Pascal Halffmann, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE
	A.46 Generalized Dominance Cones for Ordinal Optimization[2] Michael Stiglmayr, University of Wuppertal, DE	
11:20	Coffee break	

1) Plenary or track plenary, 50 min. | 2) Contributed talk, 22.5 min. (both including discussions)

11:40	**MATHEMATICAL PROGRAMMING: UNCERTAIN DATA AND MULTIPLE OBJECTIVES**	**ANALYZING MATERIALS STRUCTURES: IMAGES, MACHINE LEARNING AND STOCHASTIC GEOMETRY**
	A.07 Multicriteria Evaluation of Outsourcing Companies of Recycling and Waste Disposal[2] Nelson Hein, FURB – Universidade Regional de Blumenau, BR	**A.12 Connectivity in low porosity materials: quantification, stochastic geometry models, and relationships with material transport processes**[2] Sandra Barman, RISE Research Institutes of Sweden, SE
	A.29 Semi-infinite optimization algorithms for shape-constrained regression[2] Jochen Schmid, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE	**A.05 Copula-based modeling and simulation of 3D systems of curved fibers by isolating intrinsic fiber properties and external effects**[2] Matthias Weber, Ulm University, DE
	A.33 The single row facility layout problem with chance constraints[2] Louisa Schroeder, TU Dortmund University, DE	**A.14 Microstructure analysis using geometric and topological data analysis**[2] Yossi Bokor Bleile, Aalborg University, DK
	A.08 DEMATEL Methodology in Evaluation of Green Supply Chain Management Practices[2] Adriana Kroenke, FURB – Universidade Regional de Blumenau, BR	**A.52 Classification of materials using Topological Data Analysis**[2] Jan Felix Senge, Institute of Mathematics of the Polish Academy of Sciences, Warzaw, PL
13:10	Lunch break	
14:30	**MATHEMATICAL RESEARCH DATA**	**SIMULATION AND OPTIMIZATION IN FLUID DYNAMICS**
	A.24 Workflows for structuring mathematical research data[2] Jochen Fiedler, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE	**A.56 A second order level-set algorithm in topology optimisation and the topological state derivative (Track Plenary)**[1] Kevin Sturm, TU Wien, AT
	A.02 MaRDMO – An RDMO plugin to populate and query the MaRDI Knowledge Graph[2] Marcus Weber, Zuse Institute Berlin, DE	**A.06 Automated Solution of Shape Optimization Problems with cashocs**[2] Sebastian Blauth, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE
	A.16 Documentation of Multi-X Modeling[2] Sibylle Hermann, University of Stuttgart, DE	**A.13 Identification of Reaction Kinetics Using Gradient-Based Optimization and Lattice Boltzmann Methods**[2] Shota Ito, Karlsruhe Institute of Technology, DE
	A.58 Ontological tools and interoperability for complex materials modelling applications[2] Peter Klein, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE	
16:00	Coffee break	
16:20	**MODELS AND DATA ACROSS SCALES AND DOMAINS IN ENGINEERING APPLICATIONS**	**ANALYZING MATERIALS STRUCTURES: IMAGES, MACHINE LEARNING AND STOCHASTIC GEOMETRY**
	A.03 Physics-informed neural control of partial differential equations with applications to numerical homogenization[2] Denis Korolev, Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Berlin, DE	**A.47 3D Microstructure Image Generation using GANs with Minkowski Functionals for Fuel Cell Electrodes**[2] Abdelouahid Bentamou, Ecole des mines de Saint-Etienne, FR
	A.48 Parameter Identification by Deep Learning of a Material Model for Granular Media[2] Derick Nganyu Tanyu, University of Bremen, Centre for Industrial Mathematics, DE	**A.28 Synthetic Data for Computer Vision in Surface Inspection**[2] Natascha Jeziorski, University of Kaiserslautern-Landau, DE
	A.20 Effects from large-scale employment of model-predictive control in district heating substations[2] Henrik Håkansson, Fraunhofer-Chalmers Centre, Gothenburg, SE	**A.49 A Fast Surrogate Model for the Monto-Carlo Simulation of Electron-Matter Interaction**[2] Tim Dahmen, German Research Center for Artificial Intelligence (DFKI), Kaiserslautern, DE
	A.09 An MPC-Based Motion-Cueing Algorithm for the Robot-Based Driving Simulator RODOS®[2] Tim Nicolai, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE	**A.11 Segmenting cracks in CT images of concrete using scale invariant Riesz neural network**[2] Barisin Tin, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE
		A.44 Crack detection for 3D images of concrete using cumulative sum method[2] Duc Nguyen, Ulm University, DE
18:15	End of conference day 2	
18:30	Dinner, Atrium at Fraunhofer ITWM	

1) Plenary or track plenary, 50 min. | 2) Contributed talk, 22.5 min. (both including discussions)

Wednesday, September 27, 2023

	Auditorium	Seminar room Z03.07/08
9:00	**SIMULATION AND OPTIMIZATION IN FLUID DYNAMICS**	**MATHEMATICAL PROGRAMMING: UNCERTAIN DATA AND MULTIPLE OBJECTIVES**
	A.21 Industrial melt spinning with two-way coupled air flow including crystallization and radial effects[2] Manuel Ettmüller, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE	**A.31 Inverse shortest paths in directed acyclic graphs**[2] Orges Leka, University of Applied Sciences, Bingen, DE
	A.23 AI-based workflow for predicting and optimizing the LDDC criterion in urban areas based on Computational Fluid Dynamics[2] Jennifer Werner, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE	**A.34 Temporal Shortest Path Interdiction**[2] Alina Wittmann, Technical University of Munich, DE
	A.35 Microstructure Design and Additive Manufacturing of a Chromatography Column for the Separation of Biological Cells[2] Sonja Föhst, University of Kaiserslautern-Landau, DE	**A.27 Global solution of gemstone cutting problems using quadratic programming**[2] Tobias Seidel, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE
10:10	Coffee break	
10:30	**SIMULATION AND OPTIMIZATION IN FLUID DYNAMICS**	**JOINT SESSION: MODELS AND DATA ACROSS SCALES AND DOMAINS & ANALYZING MATERIALS STRUCTURES**
	A.17 Reconstruction of inhomogeneous turbulence based on stochastic Fourier-type integrals[2] Nicole Marheineke, Trier University, DE	**A.25 Adaptively exploring the feature space of flowsheets**[2] Michael Bortz, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE
	A.50 Positivity Preserving Time Integration Schemes for Balance Laws[2] Andreas Meister, University of Kassel, DE	**A.19 Gauss-Newton Method for ODE Optimal Control Problems**[2] Vicky Holfeld, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE
	A.51 MESHFREE: a way to ensure reliability of industrial simulations in fluid and continuum mechanics.[2] Joerg Kuhnert, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE	**A.26 Motion Estimation in Materials Science – A Mathematical Perspective to Shape and Accuracy of Calculated Displacement Fields.**[2] Tessa Nogatz, University of Kaiserslautern-Landau, DE
11:45	**Plenary A.61 Optimization: four exciting decades of progress, and a look at what the future may hold**[1] Robert E. Bixby, Rice University, Houston, Texas, US	
12:35	**Closing remarks**	
12:45	Lunch, end of conference	

1) Plenary or track plenary, 50 min. | 2) Contributed talk, 22.5 min. (both including discussions)

Information Security Visitors Rules

Binding rules during your visit:

- Visitors have to be registered when they come to the Fraunhofer institute.
- During the visit, the visitor's badge must be worn in a clearly visible manner.
- Stay with your contact person and follow the instructions of the Fraunhofer ITWM staff.
- All information is to be treated confidentially.
- Photography and video recordings are prohibited.

Notes

Notes

Abstracts

From Disruption to Success: Predictive Analytics in presence of Structural Changes in Energy systems

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In 2005, the gas market in the EU was liberalized, leading to increased market participation and shorter-term planning, making the natural gas market less predictable. In this context, the primary responsibility of Transmission System Operators (TSOs) is to meet the transport demands, ensuring the security of supply in a safe and efficient manner. As natural gas travels relatively slowly through pipes, at an average velocity of around 25km/h, it is essential to have highly accurate short to mid-term forecasts of supplies and demands to operate the complex natural gas transmission networks and distribution systems safely and efficiently. In 2022, the gas supply market in Europe, particularly in Germany, underwent significant structural changes, with the majority of supply shifting from east to west and north. To ensure the security of supply in unprecedented scenarios, TSOs had to adapt quickly and find new solutions. In this talk, we will present a robust and high-precision forecasting system developed in a joint project between Open Grid Europe, one of the largest TSOs in Germany, and Research Campus MODAL. We will discuss how the system accommodated fundamental changes in gas flow time series benefiting from underlying LP and MIP models and explore how predictive algorithms can be made even more robust and adaptive in the face of challenges.

MaRDMO
An RDMO plugin to populate and query the MaRDI Knowledge Graph

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The Mathematical Research Data Initiative (MaRDI) has set itself the goal of making information about mathematical objects, e.g. algorithms or models, available in a structured and easy-to-find manner in the form of a knowledge graph. The linking of all these objects with concrete questions, input and output data, software and hardware is done in specific workflows. To achieve reproducibility of these often interdisciplinary workflows, detailed documentation is required. For this purpose, a standardized template for workflow documentation was developed in the MaRDI project, which can be completed by answering a simple questionnaire in RDMO. Workflows recorded in this way can be stored locally or published directly on the MaRDI portal. In addition, central information of the documentations is integrated into the MaRDI Knowledge Graph. Next to the pure documentation of workflows, MaRDMO offers the possibility to retrieve existing workflows from the MaRDI Knowledge Graph in order to provide researchers with suggestions for future projects and to document workflows based on these suggestions. Thus, MaRDMO creates a community-driven knowledge loop that could help to overcome the replication crisis.

Physics-informed neural control of partial differential equations with applications to numerical homogenization

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In this talk, we discuss physics-informed neural networks (PINNs) constrained by partial differential equations and their applications in approximating multiscale PDEs within homogenization framework. From a continuous perspective, our formulation corresponds to a non-standard PDE-constrained optimization problem with a PINN objective. To provide clarity, we consider a two-scale setting, which involves a fine-scale equation at the fine scale and a coarse-scale equation at the coarse scale. We choose a neural network solver for the fine-scale problem, and it informs the coarse-scale problem through our homogenization process. This gives rise to a PDE-constrained optimization problem, which can be described as follows:

$$\begin{aligned} &\inf_{y,u_{\boldsymbol{\theta},n}} \mathcal{J}_\mu(y, u_{\boldsymbol{\theta},n}), \\ &\text{subject to:} \\ &\mathcal{L}\big[u_{\boldsymbol{\theta},n}\big] y = f, \end{aligned}$$

where $\mathcal{J}_\mu$ stands for a least-squares loss functional for the PINN problem and $\mathcal{L}[u_{\boldsymbol{\theta},n}]$ is a coarse-scale differential operator, which is informed by our neural network ansatz for the fine-scale solution. From a discrete standpoint, the formulation represents a hybrid numerical solver that utilizes both neural networks and finite elements. We present a function space framework for the problem and an algorithm for its numerical solution, combining an adjoint-based technique from optimal control with algorithmic differentiation. We show that incorporating coarse-scale information into the neural network training process through our modelling framework acts as a preconditioner for the low-frequency component of the fine-scale PDE, resulting in improved convergence properties and accuracy of the PINN method.

Large-scale statistical learning for mass transport prediction in porous materials using 90,000 artificially generated microstructures

Benedikt Prifling[1], Magnus Röding[2,3] Philip Townsend[4], Matthias Neumann[1], Volker Schmidt[1]

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Effective properties of functional materials crucially depend on their 3D microstructure. In the present contribution, quantitative relationships between descriptors of two-phase microstructures and their mass transport properties are investigated. For this purpose, a vast database comprising 90,000 microstructures drawn from nine different stochastic models is generated by using various methods from stochastic geometry. Three example structures are shown in Figure 1. For each structure, the resulting effective diffusivity and permeability as well as various microstructural descriptors are computed. To the best of our knowledge, this is the largest and most diverse dataset created for studying the influence of 3D microstructure on mass transport. In particular, microstructure-property relationships are established using analytical prediction formulas, artificial (fully-connected) neural networks and convolutional neural networks. For details, see [1]. The corresponding data is available online [2].

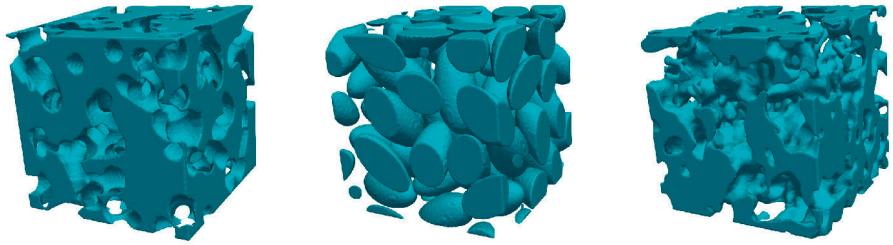

Figure 1: Simulated 3D structures generated by spatial stochastic graph model (left), hard packing of ellipsoids (center) and excursion sets of Gaussian random fields (right).

[1] B. Prifling, M. Röding, P. Townsend, M. Neumann, and V. Schmidt, "Large-scale statistical learning for mass transport prediction in porous materials using 90,000 artificially generated microstructures" *Frontiers in Materials*, vol. 8, 786502, 2021.

[2] B. Prifling, M. Röding, P. Townsend, M. Neumann, and V. Schmidt. doi:*10.5281/zenodo.4047774*, 2021.

Copula-based modeling and simulation of 3D systems of curved fibers by isolating intrinsic fiber properties and external effects

Matthias Weber[1], Andreas Grießer[2], Erik Glatt[2], Andreas Wiegmann[2], and Volker Schmidt[1]

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Fiber-based materials like, e.g., nonwovens are routinely used for various applications ranging from face masks and hygiene tissue to geological engineering, where specific properties are desirable. Stochastic fiber models facilitate the understanding of their microstructure-property relationships. We present a novel stochastic model for fibers of nonwovens which utilizes copulas to describe the evolution of a fiber. For this, we represent a fiber as an equidistant polygonal track $v_1, v_2, \ldots \in \mathbb{R}^3$ in three-dimensional Euclidean space. We model the vertices as a stationary third-order Markov chain $\{V_i, i \geq 1\}$, i.e., we give a model for the transition function $f(V_{k+1} = v_{k+1} | V_{k-2} = v_{k-2}, V_{k-1} = v_{k-1}, V_k = v_k)$ by specifying the joint probability density of $(v_1, \ldots, v_4)$. Intuitively, we assume that the shape of fibers is governed by some intrinsic properties (e.g., stiffness) and external constraints, e.g., a bounded sampling window, or preferred directions due to the production process. As fibers in nonwovens are mainly oriented within a given plane (say, the x-y-plane) we consider any deviation from that plane to be due to some external effect. Effectively, we choose a second-order Markov chain for modeling the z-components of $\{V_i, i \geq 1\}$. Moreover, by assuming stationarity and isotropy of the fiber system projected onto the x-y-plane, the behavior of the x- and x-components may be considered as intrinsic properties of fibers. For modeling these, we apply a transformation to obtain a local representation of the x- and y-components of V_1, V_2, V_3, V_4 by only 2 angles, i.e., the x- and y-components are uniquely defined by these angles up to rigid transformations of the whole fiber. Assuming independence of the z-components and modeling the described joint densities by copulas allows for a relatively simple yet powerful model. We show how the parameters of these copulas are collectively fitted to measured data and evaluate the goodness-of-fit of the resulting model. The model may then serve as a foundation for the data-driven 3D analysis of virtual fiber systems.

Automated Solution of Shape Optimization Problems with cashocs

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Even with modern hard- and software developments, the computational solution of PDE constrained shape optimization problems is still a very challenging task. There is high demand for efficient solution algorithms, particularly for complex problems arising from industrial applications. In this talk, we present cashocs, a software package which automates the solution of such problems and facilitates their efficient solution.

The software cashocs allows users to formulate their problems in a high-level language closely resembling the underlying mathematics. Moreover, cashocs automatically derives adjoint systems and shape derivatives using automatic differentiation, so that there is no more need for tedious and error-prone manual calculations. Further, this automation also makes it very easy to make modifications to the cost functional or PDE constraints without having to re-perform these calculations.

Our software implements many state-of-the-art solution algorithms for shape and topology optimization problems, such as space mapping methods for shape optimization, quasi-Newton methods for topology optimization, as well as BFGS and nonlinear CG methods for shape optimization. Additionally, cashocs provides many sophisticated methods to ensure a sufficiently high mesh quality and even has support for automated remeshing.

To highlight the capabilities of cashocs, we present several industrial applications from fluid dynamical shape optimization which are solved with cashocs. The results showcase the wide variety of highly-performant solution methods as well as the efficiency and applicability of cashocs even for very complex problems.

Multicriteria Evaluation of Outsourcing Companies of Recycling and Waste Disposal

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In the last few years, with the growing concern about the environment and the need for awareness of companies to adapt their operations to the new reality, one of the most worked-on points is waste management. From this point of view, recycling and waste disposal outsourcing companies are indispensable, as they take the responsibility of carrying out the whole process away from the producer organization and allow it to focus more on its core business, thus increasing profitability. Furthermore, companies with expertise in transportation and waste disposal already have an appropriate structure to issue all the documentation for the destination of the materials, thus eliminating the company's legal liabilities in case of environmental inspections. This paper aims to establish a methodology for outsourcing selection in the waste and recycling industry using multi-criteria decision analysis. The methods TOPSIS (Eq.1) and ADRIANA (Eq.2) were selected:

$$RCC_i = \frac{\sqrt{\sum_{j=1}^{n} w_j (v_{ij} - v_j^-)^2}}{\sqrt{\sum_{j=1}^{n} w_j (v_{ij} - v_j^+)^2} + \sqrt{\sum_{j=1}^{n} w_j (v_{ij} - v_j^-)^2}} \tag{1}$$

$$VTh_i = \frac{(m-\lambda)\sum_{j=1}^{n} w_j x_{ij} - (1-\frac{\lambda}{m})\sum_{j=1}^{n}\sum_{i=1}^{m} w_j x_{ij}}{(m-1)} \tag{2}$$

For the development of a ranking made up of 4 companies and 8 technical indicators. The indicators chosen were as follows: Financial capability (FC); capacity/interfaces (IT); Price (PR); Effective environmental management information system (ES); Quality of recycling processes (QR); Recycling capability (RC); Standardized health and safety conditions (HS); Sustainable image (SI). The scale for the valuation of the indicators used is qualitative: very bad, bad, satisfactory, good, and very good. The normalizations of the data followed the format:

$$r_{ij} = \frac{x_{ij}}{\sqrt{\sum_{i=1}^{m} x_{ij}^2}} \tag{3}$$

The weight of each indicator was obtained by the entropy of the information (Eq.4):

$$e(d_i) = -\alpha \sum_{i=1}^{m} \frac{d_i^k}{D_i} Ln\left(\frac{d_i^k}{D_i}\right) \tag{4}$$

The result of the work points out the ranking of the possible outsourcing companies.

DEMATEL Methodology in Evaluation of Green Supply Chain Management Practices

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This paper discusses the DEMATEL model for assessing the relationships among green supply chain practices, organizational performance, and external driving factors in a company. The following criteria were used for the Green Supply Chain Practices group: Green purchasing (C1)involves the formal introduction and integration of environmental issues. Green design (C2) involves environmental criteria in the product design process. Product recovery (C3) involves minimizing the amount of waste sent to landfills through material recovery or end-of-life through recycling and remanufacturing. Green information systems (C4)involve the use of information systems to achieve environmental objectives. The second group is called Organizational Performance, the following criteria were evaluated: Environmental performance (C5)reports the capability of manufacturers to reduce air emissions, waste effluent, and solid waste, and the ability to decrease the consumption of hazardous and toxic materials. Economic performance (C6) relates to the managers' ability to reduce costs associated with purchased products, materials, energy consumption, waste treatment, waste discharge, and environmental accident. Operational performance (C7) is related to the manufacturers' capabilities to produce and deliver products to customers. The third group is called External Driving Factors with the following criteria: Regulations (C8) national, governmental, and international issues. Stakeholder Pressures (C9) force companies to implement green supply chain initiatives. The following steps describe the implementation of DEMATEL: Step 1: Build the direct relationship matrix: using the linguistic scale: no influence (0); very low influence (1); low influence (2); high influence (3) and very high influence (4). Thus, the matrix $Z_k = \left[Z_{ij}^k\right]$ is built. In Step 2 the relationship matrix is normalized $X = \frac{Z}{s}$; $s = max\left(\underset{1\leq i\leq n}{max}\sum_{i=1}^{m} Z_{ij}; \underset{1\leq i\leq n}{max}\sum_{j=1}^{n} Z_{ij}\right)$. In step 3: Calculate the total ratio matrix through the equation $T = X\left(1-X\right)^{-1}$. In Step 4: a cause-and-effect diagram is calculated. In this step, the vectors R and C, representing the sum of the rows and the sum of the columns of the total influence matrix T, are defined by the following formulas:$R = \left[r_i\right]_{n\times 1} = \left[\sum_{j=1}^{n} t_{ij}\right]_{n\times 1}$ e $C = \left[c_i\right]_{1\times n} = \left[\sum_{i=1}^{n} t_{ij}\right]_{1\times n}$. The results indicate that the evaluation criteria green purchasing (C1), green design (C2), green information systems (C4), regulations (C8), and stakeholder Pressures (C9) are classified into the group of causes. On the other hand, Product recovery (C3), Environmental performance (C5), Economic performance (C6), and Operational performance (C7) are included in the effect group.

An MPC-Based Motion Cueing Algorithm for the Robot-Based Driving Simulator RODOS®

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Abstract

Interactive driving simulators have gained attention as valuable and highly efficient tools for driver training, vehicle dynamics design and development, and, last, not least, for testing of advanced driving assistance systems. To address this, Motion Cueing algorithms based on Model Predictive Control (MPC) approaches have been implemented in hexapod-based simulators. While showing reasonable results for this simulator type, its potential for robot-based simulators remains to be investigated [1–3].

This research proposes a customized MPC-based Motion Cueing algorithm for ITWM's robot-based driving simulator RODOS® to achieve a more immersive and realistic driving experience compared to conventional filter-based methods. In particular, by incorporating a model of the human vestibular system, the control of the robot can be tuned to the driver, going beyond classical washout filter-based algorithms that do not explicitly account for the subtleties of human motion perception. In this context, the choice of the model structure and an appropriate parameterization based on data is as important as the question whether and how nonlinear effects should be considered. The presented MPC framework enables the integration of advanced control strategies and predictive capabilities that provide improved motion tracking and response. Focusing on minimizing undesired platform movement inducing driver motion sickness improves comfort and overall simulator performance. A comparison with the washout filter approach already implemented in RODOS® highlights the advantages of the proposed Motion Cueing algorithm and shows a promising application of MPC in a robot-based driving simulator.

Keywords— MPC, Motion Cueing, perception modeling, driving simulation

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A 3-stage adaptive algorithm for nonlinear robust optimization

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Robust optimization deals with optimization problems under uncertainty. Two well-known approaches are min-max-regret and adjustable robustness. The idea in adjustable robustness is that not every decision has to be made right now. Some decisions can be made later when a part of the uncertainty is revealed. Therefore, the decision variable may depend on some portion of the uncertainty set. This relation is often modeled by an affine linear decision rule. Usually, in adjustable robustness the objective is to optimize for the worst case. On the other hand, in min-max-regret robustness, the objective is to minimize the maximal regret, which is the distance of the objective value for the robust solution in one scenario to the optimal objective value of this scenario. We combine elements of both concepts by using an affine linear decision rule in a min-max-regret ansatz. This gives us the flexibility to adjust our decision according to the realized uncertainty. And, the maximal regret over all scenarios is minimized, instead of optimizing for an often too conservative worst case. The combination results in a bilevel optimization problem. For solving this problem, we present a 3-stage algorithm which uses adaptive discretization of the uncertainty set via two criteria. We prove convergence results for this method and show its application to the problem of making a robust pump operation plan for a drinking water supply system with uncertain water demand.

Segmenting cracks in CT images of concrete using scale invariant Riesz neural network

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Scale invariance of an algorithm refers to its ability to treat objects equally independently of their size. For neural networks, scale invariance is typically achieved by data augmentation. However, when presented with a scale far outside the range covered by the training set, neural networks may fail to generalize.

Here, we introduce the Riesz network, a novel scale invariant neural network. Instead of standard 2d or 3d convolutions for combining spatial information, the Riesz network is based on the Riesz transform which is a scale equivariant operation. As a consequence, this network naturally generalizes to unseen or even arbitrary scales in a single forward pass.

As an application example, we consider detecting and segmenting cracks in tomographic images of concrete. In this context, 'scale' refers to the crack thickness which may vary strongly even within the same sample. To prove its scale invariance, the Riesz network is trained on one fixed crack width. We then validate its performance in segmenting simulated and real tomographic images featuring a wide range of crack widths.

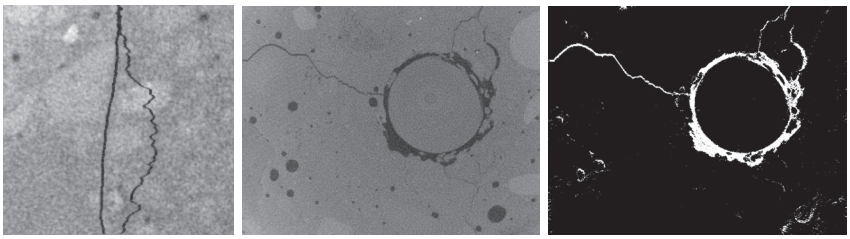

Figure 1: Simulated crack of width 3 used for training (left), real crack in concrete (center), segmentation result using Riesz network trained on crack width 3 (right).

Connectivity in low porosity materials: quantification, stochastic geometry models, and relationships with material transport processes

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Porous materials are key components in many industrial applications, such as renewable energy storage, hygiene products, packaging, pharmaceutical technology, oil recovery and C02 storage. Connecting pore geometry with material processes can aid in the development of improved materials and methods.

For low porosity materials, connectivity is a key factor determining material processes like diffusion, flow and conductivity. I will present new and existing methods to quantify connectivity. Geometric or geodesic tortuosity, which measures length of paths through the pore geometry, has been shown to have a strong relationship with transport processes. We define new methods that quantify bottlenecks caused by the pore network connectivity, termed network bottlenecks. These are bottlenecks where many paths pass through a relatively small part of the material. Network bottlenecks can greatly influence the material's properties, especially for low porosity and inhomogeneous materials.

The presented methods are useful both for summarizing the connectivity properties of a material and for exploring the connectivity visually in 3D. The methods and 3D visualization are implemented in the free software Mist [1].

I will also show a new method for stochastically generating 3D geometries with specified network bottlenecks. The method is based on thinning a pore network representation of the 3D geometry obtained from any stochastic model. Thinning is done by successively removing links while controlling for connectivity.

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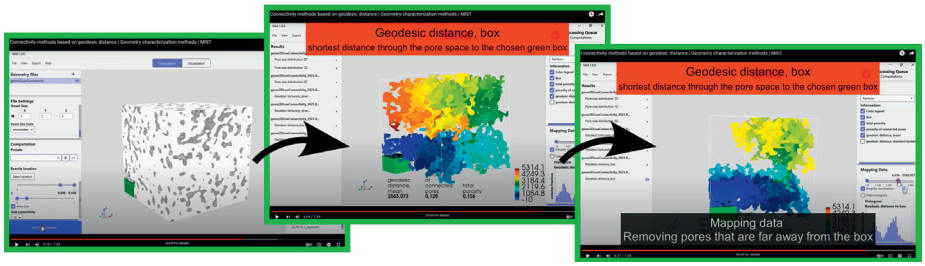

Figure 1: 3D exploration of connectivity in Mist using geodesic distance. From video tutorial at https://mist.math.chalmers.se/geodesic-distance/, where voxels with high geodesic distance are interactively removed from the visualization.

Identification of Reaction Kinetics Using Gradient-Based Optimization and Lattice Boltzmann Methods

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Understanding and improving chemical reaction processes generally necessitate quantitative information about the kinetic parameters, e.g., reaction constants and reaction orders. However, their identification often requires multiple experiments making it a challenging and resource-demanding process. In our study, we utilize computational fluid dynamics (CFD) and optimization methods to identify kinetic parameters from partially given or noisy reactant concentration distributions. Therefore, gradient-based optimization methods minimize the difference between the simulated concentration distribution and the given dataset by adjusting the kinetic parameters iteratively. The simulation is conducted with a Lattice Boltzmann Method (LBM), solving the reaction-advection-diffusion equation, coupled with a Navier-Stokes equation, to model the reactive fluid flow. The chosen LBM and the optimization algorithms are implemented in the open-source library OpenLB. A benchmark test case confirms the applicability and validity of the presented method using CFD simulations with a priory known sets of kinetic parameters, which are recovered reversely.

Microstructure analysis using geometric and topological data analysis

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In [8], persistent homology is applied to medium-range order (MRO) glass structures, to characterise static structures and their porosity. This is of interest, as various properties and functionalities of materials are influenced by the porosity of the material's structure. Understanding the relationship between the structure and the proprieties/functionalities is an important aspect in the design and production of new materials, in particular functional materials for a sustainable society. The porosity of a material is a particularly important structure, which can influence gas separation and storage ability of nanoporous materials[1, 5, 7], mechanical deformation and strength[3, 4], internal diffusion of ions or gases[6, 9]. Control of the generation, annihilation, and redistribution of free volume is thus important for the rational design of new functional materials for a sustainable society.

Various computational techniques have been employed to map out the possibilities of controlling material porosity and identify promising candidates for various applications. The typical descriptors of free volume are surface area, largest included sphere, etc. However, these do not provide sufficient geometric information to distinguish materials with different pore shapes (e.g., tunnels vs. voids)– a particular problem for amorphous materials, in which the lack of long-range structural order gives rise to a distribution of pore shapes. Hence, we are exploring the use of tools from geometric and topological data analysis to understand the difference in pore shapes and their relation to the properties of the material.

Similar tools can be applied to images of human mesenchymal stem cells (hMSCs), to characterise their growth patterns and structures [2]. In this case, persistent homology is used to obtain a topological summary of the morphology of cells, which we use to calculate a 'dissimilarity score' between pairs of hMSCs. Using standard clustering techniques, we can identify sub-populations exhibiting different growth patterns. In fact, these sub-populations allow us to detect cells that are 1) not hMSCs (due to the collection procedure, about 5% of cells are not hMSCs) or 2) have issues in their imaging/data processing.

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Concurrent two-scale simulations in solid mechanics with Deep Material Networks

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Microstructured materials fit the needs of many industrial components due to their favorable mechanical properties. However, their microscopic constitution needs to be accounted for when the inelastic behavior needs to be accounted for when designing industrial components. Deep Material Networks (DMNs), originally introduced by Zeliang Liu and co-workers, offer a deep-learning based multiscale strategy which combines mathematical robustness, computational efficiency and engineering accuracy.

DMNs are based on hierarchical laminates and are trained either on linear elastic data or on quick-to-evaluate inelastic constitutive laws and applied to sophisticated inelastic material behavior. Thus, they inherently synthesize training data and sophisticated constitutive models.

The talk at hand will discuss the basics of DMNs and recent improvements for industrial problems, highlighting the remaining challenges and opportunities.

Documentation of Multi-X Modeling

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Research data management involves the organization, documentation, storage, and sharing of research data and software to ensure their accessibility and usability for subsequent use. In the context of the NFDI (National Research Data Infrastructure in Germany) consortia, ontologies and subject-specific metadata are developed to facilitate data discovery, interoperability, and reuse. In MARDI (Mathematical Research Data Initiative), one focus is on describing mathematical models that can be used across disciplines and understood by researchers with different backgrounds. The Cluster of Excellence SimTech is an example of interdisciplinary data-driven simulation, which uses multi-X modeling to simulate complex systems. Multi-X modeling includes modeling spatial and temporal scales of various orders, a wide range of coupled physical phenomena, fluids, and materials, and different modeling approaches. Additionally, it deals with heterogeneous data fidelity and faces widely different demands on output dimensionality and response. At the core of research data management are always the FAIR (Findable, Accessible, Interoperable, and Reusable) principles, focusing mainly on metadata, but not answering what information is essential for documentation. One challenge in using multi-X modeling is the reuse of existing models. Often, researchers need to use models from other domains without having expertise in those domains. Metadata are helpful in finding relevant models, but more information is needed to reuse them effectively. To make the simulation process reusable, it has to be documented adequately. However, the question is, what should be documented?

To address this question, we look at approaches from philosophy of science and how they can be applied to multi-X simulations. We conduct a case study to evaluate the concepts of epistemology, emergence, as well as validation and verification and their consequences for documentation on a concrete example. Epistemology examines the process of knowledge acquisition, and emergence the interaction of the parts with the whole system. To establish the credibility of the simulation, the two principles of verification and validation are used. Verification focuses on internal consistency and logical coherence within a theoretical framework, while validation examines the correspondence between scientific claims and empirical evidence.

In the case study, we found that underlying decisions are not documented in articles nor in the research data, which makes it difficult to understand the research. Additionally, the coupling of the model and the model as a whole was not documented. By applying the concepts of epistemology, emergence, validation, and verification to multi-X modeling, we can develop a more comprehensive and systematic approach to documenting the simulation process, to ensure that the simulation process is properly documented and can be verified.

Reconstruction of inhomogeneous turbulence based on stochastic Fourier-type integrals

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Turbulence is a continuum phenomenon. A turbulent flow field exhibits random variations in space and time. These fluctuations arise from the motion of vortices and are distributed over all wave lengths due to the mechanism of vortex stretching: the largest vortices depending on geometry and boundary conditions receive their energy directly from the mean motion and give it to the smaller vortices. The smallest vortices dissipate into heat due to viscosity.

In statistical turbulence modeling, the turbulent flow velocity is considered as a random field in space and time, usually split into expected value (mean velocity) and centered fluctuations. The fluctuations are characterized by the kinetic turbulent energy and the dissipation rate with the kinematic viscosity of the flow. Statistical turbulence models, such as, e.g., the k-ϵ-model based on the Reynolds-averaged Navier-Stokes equations with constitutive laws, provide these quantities. However, they do not describe the fluctuations themselves, which would be desirable for many applications in the field of fluid-structure interactions, such as particle dynamics.

In this talk we present a reconstruction of inhomogeneous turbulence based on stochastic Fourier-type integrals. The reconstruction satisfies the characteristic flow properties in terms of kinetic energy and dissipation rate, yields ergodicity, and enables efficient numerical simulation based on (stochastic) quadrature rules.

Active Learning of Surrogate Models for Inverse Problems

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In tasks where many similar parameter identification problems must be solved, such as quality control or nondestructive testing, inversion methods based on computationally expensive forward models are impractical. Replacing the forward model by a cheap surrogate model, such as Gaussian Process Regression, is attractive.

While in such an online-offline decomposition the computational resources available for generating training data are large, they are still bounded. We consider the design of computer experiments problem of selecting a suitable number of training data points, their position in the parameter space, and their forward model simulation accuracy for a given computational budget.

Based on work models for the simulation accuracy given some tolerance, and accuracy models for the parameter identification error given some surrogate model accuracy, we consider a theoretically backed greedy strategy for a close to optimal choice of the computational design. We show a significant efficiency improvement over a priori designs such as latin hypercube or low discrepancy sequences as well as over position-adaptive designs at some numerical examples, demonstrating the importance of taking simulation accuracy into account for the efficient generation of simulated training data. We also apply the proposed method to problems in optical metrology, reconstructing geometric parameters of nanophysical structures. The experimental results demonstrate both efficiency of the setup and effectiveness of the surrogate model, allowing for successful reconstruction with a high degree of accuracy[1,2].

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Gauss-Newton Method for ODE Optimal Control Problems

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In this talk, we present a solution method for optimal control problems with an ordinary differential equation (ODE) and tracking objective. The goal is to compute control or input functions as well as, possibly, uncertain model parameters for a dynamical system given by an ODE.
Such problems arise, e.g., in specific inverse tracking problems in vehicle engineering [1]. The goal is to infer input or excitation signals for system simulation based on measured output reference signals. For instance, the quarter-car (suspension) model requires the road profile as input to simulate the displacements of the lower and upper body masses, velocities of those or resulting forces.
There exist several different solution approaches from classical ODE optimal control theory that can be classified in *first-discretize-then-optimize* and *first-optimize-then-discretize*, for more details see [2]. Here, we propose a non-standard solution approach of the latter type and consider the ODE optimal control problem as an infinite-dimensional optimization problem, for which a Gauss-Newton method in a suitable Banach space setting is applied.
In the proposed Gauss-Newton approach, an iterative procedure is applied to the tracking problem, where in each iteration step one solves a linearization of the problem, i.e., a linear surrogate model around the current iterate is considered. The resulting linear auxiliary problem has the form of a linear quadratic ODE tracking problem that is solved via the Gradient Descent method in function spaces, or a Riccati-based method, respectively.
We discuss the proposed approach, also in comparison with classical techniques for ODE optimal control problems, and illustrate the method with numerical studies.

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Effects from large-scale employment of model-predictive control in district heating substations

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With the introduction of advanced methods for controlling the heat demand of district heating substations, such as model predictive control (MPC), different objectives of the control can be varied while still ensuring a comfortable indoor climate to very good precision. This new control regime increases the importance of the supplier's price model, which implicitly dictates the incentives of the control and may thus affect the system heat load even at an hourly level. We study the system effects of varying implementations of price models by simulating optimal heat control for populations of dwellings and workplaces, where a comfortable climate is required only within certain hours for the latter. The results suggest that both the consumption and the peak load of the entire system may be reduced by going from traditional weather-compensated control to MPC, especially if incentives given by the pricing model are appropriately tuned. We also show that by employing one common MPC for multiple buildings simultaneously, the accumulated consumption in the system and the peak loads can be reduced even further with optimal scheduling.

Industrial melt spinning with two-way coupled air flow including crystallization and radial effects

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Fiber melt spinning is one of the most important manufacturing processes in the production of technical textiles. Polymer melt is extruded under pressure through hundreds of small orifices into a spinning duct and drawn down by a take-up roller. The resulting liquid jets are cooled down and stretched during the process. In the case of semi-crystalline polymers, crystallization occurs along the spinline, which has a significant effect on the properties of the final product. Experiments have shown that the degree of crystallization is thereby not homogeneous across the cross-section of the fiber. This means that both crystallization and radial effects need to be taken into account in order to accurately model the melt spinning process.

In terms of modeling and simulation we are faced with a complex multiphase-multiscale problem due to the need to take into account the fiber-airflow-interaction as well as the consideration of the size of an industrial spinning device compared to the slender fibers. Therefore, a direct three-dimensional simulation of the process will not be feasible.

In this talk, we present a two-way coupled simulation framework that combines airflow with fiber simulations through an actio-reactio-principle. The main focus is on the fiber simulations as the airflow simulations are performed with commercial software. For the fiber simulation, a viscoelastic two-phase model is used which is capable of predicting radial temperature and crystallinity profiles along the spinline. The resulting one- and two-dimensional model equations are solved by an efficient solution algorithm which allows the iterative coupling between airflow and fibers in an acceptable time window. This opens the field for simulation-based process design and material optimization.

A certified adaptive surrogate hierarchy for parametrised reactive flow[1]

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Within the BMBF project (05M20PMA) on *Maschinelles Lernen und Modellordnungsreduktion zur Vorhersage der Effizienz katalytischer Filter*, we developed a hierarchy of surrogate models in the context of reactive flow, based on projection-based Reduced Basis reduced order models as well as machine-learning based surrogates like Kernel methods or artificial neural networks. The key contribution in [1] was to use each model in the hierarchy to generate training data for the next. While [1] still relied on a traditional separation of the computational process into a training and prediction phase (or offline and online phase), we recently enabled certification of the machine-learning based surrogates which allows for an adaptive model hierarchy that is trained on-demand during evaluation without any manual input [2]. We demonstrate this adaptive model hierarchy in the context of PDE-constrained optimisation for reactive flow.

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AI-based workflow for predicting and optimizing the LDDC criterion in urban areas based on Computational Fluid Dynamics simulations

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Wind conditions can be not only uncomfortable but also unsafe for pedestrians and residents of urban areas. A new building has a significant impact on the wind behaviour. Due to tall buildings and wind tunnel effects between buildings, strong winds can occur at street level. To counteract this, it is important to carry out wind simulations before new buildings are built. This is considered an important issue by many municipal authorities when planning new buildings in a city. For this reason, the use of generative design software in the early stages of planning new buildings in urban areas is becoming increasingly important. In order for a planning tool to be practical in the early design phase, the performance feedback of such software is an important, but still critical factor.

In the proposed work we assume that a new building complex consisting of multiple segments is constructed at a fixed location, and present an AI-based workflow to predict and optimize wind comfort (LDDC criterion). A Deep Learning model trained on simulation results by the immersed-boundary flow solver IBOFlow to predict total velocities is used as a surrogate model for the optimization process. For the calculation of the LDDC criterion, it is necessary to simulate different wind directions and evaluate them with respect to a wind rose statistic. We propose an augmentation strategy to train the surrogate model independently of a specific wind rose statistic. Using the surrogate model, we can predict the LDDC criterion with an average F1–score of 84.39 % based on only 167 simulations.

In the optimization process, the objective is to maximize the wind comfort in a given use case area so that the constraints (minimum/maximum number of floors) are respected for each segment of the building complex. We use the gradient-free solver COBYLA for this task, which takes about 200 steps to solve the optimization problem. If we had performed the optimization with the CFD solver, we would have had to run 200 individual simulations. Each simulation takes about 5 days for the specific use case, resulting in a total time saving of 1000 days (about 2.74 years). In reality, a designer of a new building would never be able to explore the solution space as it takes too much time to run the simulations. Therefore, the use of a surrogate model in the planning process seems promising.

Workflows for structuring mathematical research data

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In the mathematical sciences, a large amount of data is regularly generated. This includes numerical data used and produced for specific computations, but also information of models, calculation methods, software, notations, etc. While there is now a growing awareness of the need to make numerical data findable, accessible, interoperable and reusable (FAIR), this awareness is not yet very pronounced for the other mentioned forms of data that arise. However, the research community can also benefit greatly for precisely these forms of data if they are stored according to FAIR principles, as we will explain in our talk.

As part of a solution approach, we present and discuss first results obtained by the interdisciplinary working group of the mathematical research data initiative (MaRDI) [1], which enable a fair storage of information on used workflows and models. In the process, the potentially complex work processes are recorded in a structured manner in a workflow schema. It combines a description of what is done with auxiliary information like software and hardware used as well as the applied mathematical models and solution techniques, and algorithms with their corresponding properties. Within MaRDI, the standardized workflow documentation template MaRDMO is developed [2] which helps to document the potentially complex workflows a researcher may be involved in. For the models that are used in research, we develop an ontology, which allows to classify single components and quantities and to implement a knowledge graph that can then be browsed via a web platform. In this way, a wide variety of models and problems are linked together so that researchers can identify connections between different applications and exploit possible synergies.

The concepts designed so far are demonstrated on specific use cases involving complex mathematical models, parameter identification and data acquisition. They originate from applied research and therefore touch on diverse areas of mathematics, such as modeling, optimization, statistics, or machine learning - they are therefore not limited to a specific area of mathematics. The gains of documenting research data in such a scheme are compared to the expected additional effort.

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Adaptively exploring the feature space of flowsheets

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Simulation and optimization of chemical flowsheets rely on the solution of a large number of non-linear equations. Finding such solutions can be supported by constructing machine-learning based surrogates, relating features and outputs by simple, explicit functions. In order to generate training data for those surrogates computationally efficiently, schemes to adaptively sample the feature space are mandatory. In this contribution, we present a novel family of utility functions to favor an adaptive, Bayesian exploration of the feature space in order to identify regions that are convergent, fulfill customized inequality constraints and are Pareto-optimal with respect to conflicting objectives. The benefit is illustrated by small toy-examples as well as by industrially relevant chemical flowsheets.

Motion Estimation in Materials Science – A Mathematical Perspective to Shape and Accuracy of Calculated Displacement Fields.

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Estimating motion from images is an ill-posed problem. Nevertheless, assessing the change between images of time series is vital in many areas, such as autonomous driving or assessing tumor growth in medical image data. Another area where estimating motion from images has turned our to be very beneficial is materials science. In so called in situ tests one applies a mechanical test to a specimen and acquires X-ray computed tomography (CT) images in parallel.

The ill-posedness of motion estimation originates from the fact that the number of unknowns exceeds the number of data points by far. Take for example the case of pixelwise (or voxelwise in 3D) estimation of a displacement vector field. That means, one aims at calculating displacement $\mathbf{u}\colon \mathbb{R}^3 \to \mathbb{R}^3$ from two images $I_0, I_1\colon \Omega \subset \mathbb{R}^3 \to \mathbb{R}$, such that

$$I_0(\mathbf{x}) = I_1(\mathbf{x} + \mathbf{u}(\mathbf{x})) \tag{1}$$

is fulfilled. In this case, one tries to estimate a three dimensional quantity from only scalar correspondences. The theory of inverse problems proposes so-called regularization to tackle this problem. That means, we transform the above equation into a minimization problem and pose additional regularity constraints to guarantee existence and uniqueness of solutions. One tries to solve

$$\min_{\mathbf{u}} ||I_0(\mathbf{x}) - I_1(\mathbf{x} + \mathbf{u}(\mathbf{x}))||_p + \mathcal{R}(\mathbf{u}), \tag{2}$$

with $p = 1, 2$. $\mathcal{R}$ is the regularization operator, often defined by a (half-)norm of a certain function space. Not only the choice of p but especially the choice of $\mathcal{R}$ has crucial influence on the shape of a solution $\mathbf{u}$. Whereas in medical purposes often strong differentiability of the displacement field is assumed, computer vision experienced the triumph of total variation. Motion estimation approaches stemming from material scientists on the other hand often aim to stay close to outcomes and principles of (finite element) simulations.

In this talk, we present the state-of-the-art algorithms in 3D motion estimation from medicine and materials science. We display how the different solution approaches require certain function spaces and demonstrate the mathematical and real-life consequences on computed displacement fields. We also show how extensions of classical 2D methods to 3D perform significantly better than established methods in the field of materials science. We finish the talk with a novel strategy that addresses a further, material science specific challenge, namely the applicability to large datasets.

Global solution of gemstone cutting problems using quadratic programming

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In gemstone cutting, a rough gemstone is given. This rough stone needs to be processed. It does not have an attractive shape and has defects such as cracks and inclusions that need to be removed. This rough stone can be considered as a container. Inside the container a nice gemstone has to be embedded that makes the best use of the raw material. We consider three different types of parameters that describe the embedded gem: the position, the size, and the rotation.

The rotation introduces non-convexity into the optimization problem. So far, the problem has been studied using local approaches. Globalization has only been achieved using multi-start strategies. In this talk we want to describe a new strategy that can be used to guarantee the global solution of the problem. We describe the scaling and rotations in three dimensions using quaternions. The resulting problem can then be described as a quadratic optimization problem, which we solve to global optimality.

In recent years, several branch-and-bound solvers have been developed and extended to handle quadratic constraints and a quadratic objective. Using the developed quadratic problem, we compare the performance of these solvers. We then discuss various strategies, such as symmetry breaking and row generation that further improve the performance of the global optimization.

Synthetic Data for Computer Vision in Surface Inspection

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Manufacturing processes require fast and precise quality inspection, introducing the need for automated inspection systems. The intricate complexity of product geometry and fast evolving production methods make traditional computer vision methods unreliable and cumbersome due to low flexibility. On the other hand, the deep learning paradigm depends on a large quantity, variety and balance of data which is slow and expensive to obtain in the real-world. To overcome the data problem, we explore the usage of synthetically generated data using CAD models of products and modelling both the defect geometry and surface texture. This enables us to generate large amounts of data with controlled variety without the need to collect sufficient amount of data from the production line.

We focus on metallic products processed either by sandblasting or face-milling and restrict on modelling their surface texture. Both processing methods produce significantly different surface topographies. Thus, separate models are needed each with varying amount of deterministic and random components. Sandblasted surfaces are stationary having almost no deterministic part. In contrast, face-milled surfaces show the characteristic ring-shaped pattern caused by the tool's circular movement. Here, process-induced parameters exist but additional randomness is needed to prevent a completely deterministic pattern. Using physically based rendering of the synthetic objects we obtain images similar to those obtained by the inspection system.

Deep models trained purely on synthetic data show somewhat lower performance compared to training on a subset of the available real data due to approximations in the simulated inspection environment. However, fine-tuning on a small subset of real data greatly increases the model performance demonstrating that synthetic data supports model training. Having a digital twin of the inspection environment allows us to more easily design inspection plans even before interaction with the physical inspection acquisition setup.

We continue to explore the abilities of procedural models across different products, defects and acquisition scenarios to support fast and reliable design of inspection setups for the industry.

Semi-infinite optimization algorithms for shape-constrained regression

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We present adaptive discretization algorithms for shape-constrained regression. In shape-constrained regression, one tries to learn a model such that, on the one hand, it optimally fits the given data and, on the other hand, it satisfies certain shape constraints known about the true relationship to be modeled. In many cases, such shape-constrained regression problems can be cast as convex semi-infinite optimization problems. In particular, this is true in the case of monotonicity or convexity constraints which frequently occur in engineering applications. We present an adaptive discretization algorithm tailored to such problems. It terminates after finitely many iterations at a feasible point, that is, at a model that strictly complies with all the imposed shape constraints. Additionally, the optimality error of the computed feasible point can be bounded above in terms of the approximate-solution tolerances of the finite subproblems of our algorithm. We discuss several applications of our algorithm to concrete engineering applications, like glass bending, press hardening, brushing, and milling.

Dynamic Human Body Models in Vehicle Safety: An Overview

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Significant trends in the vehicle industry are autonomous driving, micromobility, electrification and the increased use of shared mobility solutions. These new vehicle automation and mobility classes lead to a larger number of occupant positions, interiors and load directions. As safety systems interact with and protect occupants, it is essential to place the human, with its variability and vulnerability, at the center of the design and operation of these systems. Digital human body models (HBMs) can help meet these requirements and are therefore increasingly being integrated into the development of new vehicle models. This talk provides an overview of current HBMs and their applications in vehicle safety in different driving phases from stationary over low and high dynamic driving to accident phases, see Fig. 1. The speaker briefly introduces the underlying mathematical models, methods and caviats and presents two case studies to improve understanding and product development in the field of vehicle safety:

- In-crash finite element simulations and injuries of riders on a motorcycle.
- Prediction of human behavior in take-over scenarios.

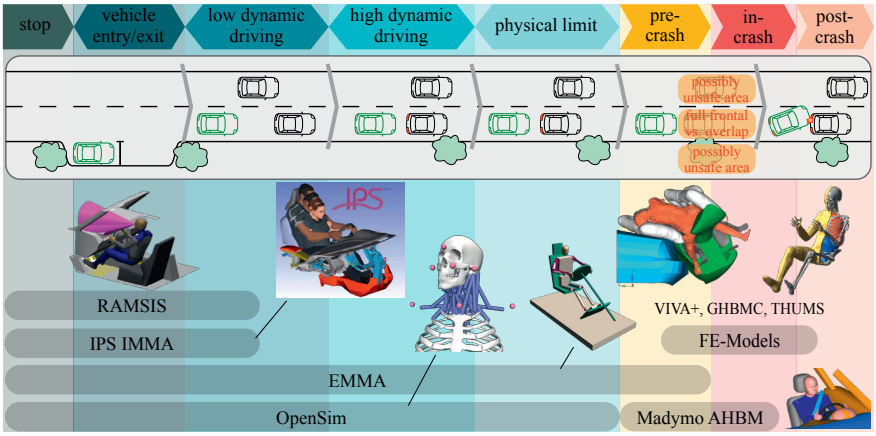

Figure 1: Exemplary human body models (HBMs) for different driving and accident phases.

Inverse shortest paths in directed acyclic graphs

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The inverse shortest paths problem introduced 1992 by Burton and Toint deals with determining the costs on edges that give rise to given shortest paths on a given directed graph. In this paper, we explore the problem of finding edge costs that explain the given shortest paths on a directed acyclic graph and present a heuristic for solving this problem.

Furthermore, we introduce the idea of considering directed acyclic graphs with a topological ordering and representing this ordering on a line, which can be interpreted as a shortest path in the plane. Each path with nodes on this line is then a shortest path if we consider the distances on the line between the nodes as the new edge weights.

Overall, this paper presents a formulation and heuristic algorithmic approach to solve the inverse shortest paths problem on directed acyclic graphs. It introduces the concept of using lines to represent topological orderings and demonstrates the applicability of the proposed method in finding edge costs that explain given shortest paths while minimizing the l_2-norm with respect to the original costs.

The proposed heuristic is faster then solving the original problem of Burton and Toint, and can be extended, using the kernel trick, to directed acyclic graphs G with a positive definite kernel k on the nodes V of the graph, which could make it attractive for applications, where the measured costs betweeen two nodes on the graph, could be flexibly determined by different positive definite kernels k.

Applying Reverse Search Enumeration to Tri-Objective Linear Programming: A New Way to Parallelize Finding Extreme Points

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In multi-objective optimization, we are interested in the set of non-dominated points. The set of non-dominated extreme points is a special subset, for many problems it is much more practical to enumerate the extreme points instead of all non-dominated points.

An algorithm to enumerate this set was developed by Bökler in 2022. His algorithm is the first polynomial-delay algorithm for tri-objective linear programming (TOLP). We build upon his approach and devise a new algorithm to find extreme points for TOLP. Our algorithm adapts the well-known reverse search enumeration technique. Through this, we loose the polynomial delay of Bökler's algorithm but instead we gain a polynomial space algorithm. Furthermore, this new algorithm allows a straight-forward parallelization. This marks an important development, as the current state-of-the-art algorithms are notoriously hard to parallelize.

We conduct a computational study on our algorithm and compare the performance of our implementation to an implementation of Bökler's algorithm and the two current state-of-the-art solvers BENSOLVE and PaMILO. The results show that there are still some obstacles to overcome in practice. But at the same time, they highlight the potential of the new algorithm to archive a significant speed-up through parallelization.

The single row facility layout problem with chance constraints

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In the single row facility layout problem (SRFLP) machines are arranged in a plant floor along one side of a path without overlapping. The aim is to minimize the handling costs of the material, which are represented as the sum of the pairwise distances between the machines weighted with the costs of the material flow.
The majority of the literature assumes complete knowledge of the input data for the SRFLP. In real life scenarios the input data is unknown beforehand and the predictions may underlie fluctuations. Therefore, it is reasonable to take uncertainty of the input data into account.
In this talk we present a new version of the SRFLP by using chance constraints to consider variations in the material flow between the machines. We assume that the material flow follows a multivariate normal distribution. We present preliminary results.

Temporal Shortest Path Interdiction

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Network interdiction problems deal with the question of how the optimal objective value of an optimization problem on a graph or network (e.g., a shortest path or network flow problem) can be worsened as much as possible by removing a limited number of arcs. These problems represent an important research topic and have a variety of practical applications such as assessing the robustness of critical infrastructure networks or containing the spread of infectious diseases.

In many of these applications, however, the underlying graph is not static, but each arc is active only at a specific point in time. For example, train connections in a passenger transportation network are only available at specified departure times, and in the case of infectious disease spread, contacts between individuals exist only at specific times. The graphs that appear here, where the set of active arcs changes over time, are called temporal graphs in the literature.

In this talk, we connect network interdiction problems and temporal graphs by investigating the interdiction of shortest paths in temporal graphs. The resulting temporal shortest path interdiction problem generalizes one of the most important network interdiction problems to temporal graphs. It studies the question of how to remove a bounded number of arcs from a temporal graph such that the length of a shortest path between two given nodes is maximized. We characterize the complexity of the temporal shortest-path interdiction problem for various natural interpretations of "shortest" paths in temporal graphs (latest start path, earliest arrival path, shortest duration path, shortest traversal path). Although the static shortest path interdiction problem is known to be NP-hard, we obtain polynomial-time algorithms for two of the four problem variants. Finally, we give an outlook on further interesting research topics on network interdiction problems in temporal graphs.

Microstructure Design and Additive Manufacturing of a Chromatography Column for the Separation of Biological Cells

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The separation of biological cells (cell chromatography) plays a crucial role in many processes in biotechnics. For example, it is of central importance in stem cell research or blood cancer therapy. The current separation procedures are based on complex, sometimes multi-stage process chains.

To simplify this procedure, we aim for an in-flow cell separation, which significantly simplifies the process of cell separation. The separation medium is produced using high-precision additive manufacturing processes. Afterwards, it is placed in a glass column through which a cell-enriched suspension flows.

Within our research, we virtually develop such a separation medium using mathematical modeling and simulation. We consider foams based on Laguerre tessellations. Their numerous parameters allow for a high degree of flexibility regarding the structural properties. Parameters such as the size of foam pores or the thickness of foam struts can easily be adjusted to enable the best possible separation of the biological cells. Constraints required by the microscale manufacturing process such as minimal structure thickness can be fulfilled.

The separation of living cells is attempted by the use of a functionalized surface. Therefore, a mathematical model has to account for the interaction of cells with the functionalized surface. A classical particle movement model was extended with additional forces and a special contact model. With the help of this model, the developed structures can be rated in terms of separation efficiency and resulting pressure drop.

During our talk, we present the modeling of the separation medium as well as the cell-interaction model.

With our approach, a wide range of structures can be evaluated and analyzed with relatively little effort. Once an optimal structure is found, the separation medium will be manufactured and evaluated within real cell separation scenarios.

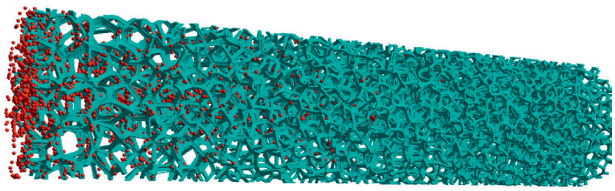

Figure 1: Foam structure in light blue and deposited cells in red

Comparison of different image representations and their suitability for classification of material microstructures by machine learning

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For several years already, machine learning (ML) has been able to achieve outstanding results in the classification and segmentation of materials microstructures and can be used successfully in particular for high-performance materials with their increasingly narrow microstructural tolerances. While initially conventional ML algorithms (e.g., support vector machine, random forests) with prior feature extraction by an expert were predominantly used, a strong trend towards the use of deep learning (DL) can be observed over the last few years. Conventional ML has the advantages of working with smaller amounts of data and being more interpretable, while the convolutional neural networks used in DL learn not only the classification but also the feature extraction by itself. With a new task of classifying microstructures, the question then naturally arises whether it is better to use conventional ML or DL. Based on two examples of steel microstructures, this work presents different image representations and systematically compares the classification by conventional ML and DL. The efforts of feature engineering (incl. feature selection) for conventional ML are examined, generalization and interpretability of ML and DL are compared and for DL also the domain gap between the usually performed ImageNet pretraining and microscopic microstructural images is discussed.

Finite representation of quantile sets for multivariate data via vector linear programming

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A well-known result states that empirical quantiles for finitely distributed univariate random variables can be obtained by solving a linear program. We show in this short note that multivariate empirical quantiles can be obtained in a very similar way by solving a vector linear program. This connection provides a new approach for computing Tukey depth regions and more general cone quantile sets.

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Exploring the Optimal Camera Placement Problem and its Relationship with the Set Covering Problem

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Optimal Camera Placement (OCP) is the process of finding the optimal locations and orientations of a set of cameras, where the objective can be to maximize the coverage of a given surveillance area or minimize the total cost of the selected cameras. This should be achieved while ensuring that a given set of constraints such as specific point coverage, camera budget, camera quantity, and other case-specific restrictions, are satisfied. In some studies, this problem has been formulated in a way that resembles the formulation of the Set Covering Problem (SCP). This similarity has not been explicitly discussed in the literature until recently. Therefore, this paper studies the OCP problem by exploring its literature and understanding its relationship with SCP. Furthermore, the aim of this study is to find techniques from the SCP literature that can be used to deal with the OCP problem. More specifically, this study focuses on exploring a variety of instance reduction techniques that were studied in the SCP literature to reduce the size of a problem. Since OCP is an NP-hard problem, which means it can be time consuming to solve some large instances using exact methods, reducing its size can significantly reduce the amount of time needed to provide optimal solutions. This study proves this by providing a comparison between the results of some instances and the reduced version of these instances. For future work, this OCP problem could be formulated as a multi-objective problem, where the main objectives are maximizing the coverage and minimizing the total camera cost. There are several techniques that have been mentioned in the multi-objective SCP literature, which can be used to deal with the multi-objective OCP problem. This paper discusses such techniques and explores potential objectives that can be added to the OCP problem.

The Weighted p-Norm Weight Set Decomposition for Multiobjective Discrete Optimization Problems

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Scalarization is a widely used technique that transforms a multiobjective programming problem into a scalar-valued optimization problem to obtain an efficient solution or nondominated image. Two well-known scalarization techniques are the weighted sum and weighted Tchebycheff scalarization. Both can be interpreted as a weighted p-norm scalarization: a positive weight is applied to each objective function, and the distance to a given reference point is minimized under a p-norm.

For the weighted sum and weighted Tchebycheff scalarizations, the set of eligible weights has been studied with a successful application of a weight set decomposition approach: the set of eligible weights is divided into subsets such that all weights in a subset give the same image of an optimal solution under the objective function. In doing so, the structure of the set of eligible weights is linked to the structure of the set of images, providing additional information, such as robustness and adjacency of images. Therefore, the understanding of the structure of the weight set decomposition is particularly useful as an additional support for a decision maker when selecting their most preferred solution or image.

We apply the weight set decomposition approach to general weighted p-norm scalarizations, generalizing and complementing existing results for the weighted sum and weighted Tchebycheff scalarizations.

Scenario generation for market risk models using generative neural networks

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The calculation of market risk in accordance with Solvency II in an internal model is currently mainly performed using a Monte Carlo simulation, in which scenarios of financial market developments over a period of one year are derived using an economic scenario generator (ESG). The individual financial market risk factors are modeled by means of stochastic differential equations and their dependence on each other is represented by correlation matrices, joint processes or copulas. As an alternative, a special architecture of two neural networks, called "generative adversarial network" (GAN), is investigated in this research. This approach has the advantage of not requiring financial-mathematical assumptions and of accurately representing joint distributions.

Currently, there is no standard measure for evaluating the quality of these scenarios generated by a GAN. For validation of this approach as well as for optimization of GAN architecture, we provide a consistent, data-driven framework using existing evaluation measures based on nearest neighbor distances and a newly developed measure for the detection of the memorizing effect.

Based on this, a GAN is developed that can model the full band-width of investments for an insurance company and for a one year time horizon as required in Solvency 2. We demonstrate that the results of a GAN-based ESG are similar to regulatory approved internal models in Europe when using the portfolios from the "market and credit risk comparative study" of the European regulator EIOPA as benchmark portfolios. Therefore, GAN-based models can be seen as an assumption-free data-driven alternative way of market risk modeling.

Calculating Expectiles and Range Value-at-Risk using Quantum Computers

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Risk measures are important key figures to measure the adequacy of the reserves of a company. The most common risk measures in practice are Value-at-Risk (VaR) and Expected Shortfall (ES). Recently, quantum-based algorithms are introduced to calculate them. These procedures are based on the so-called quantum amplitude estimation algorithm which lead to a quadratic speed up compared to classical Monte-Carlo based methods.

Based on these ideas, we construct quantum-based algorithms to calculate alternatives for VaR and ES. These alternative risk measures are the so-called expectiles and the Range Value-at-Risk (RVaR). We repeat their desirable properties and explain the construction of our quantum algorithms. These algorithms are also based on amplitude estimation. In a case study, we compare their performance with the quantum-based algorithms for VaR and ES. We find that all of the algorithms perform sufficiently well on a quantum simulator. Further, the calculations of expectiles and VaR are robust against noise on a real quantum device. This is not the case for ES and RVaR.

Fatigue detection from sequential testing of biomechanical data using martingale statistic

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Injuries to the knee joint are significantly high for long-distance and frequent runners. We address the problem of fatigue detection in biomechanical data, consisting of lower extremity joint angles and ground reaction forces from running athletes. This is done by sequentially testing for change in a datastream using a martingale test statistic. Time-uniform probabilistic martingale bounds are provided which are used as thresholds for the test statistic. Sharp bounds can be developed by a hybrid combination of piece-wise linear- and a law of iterated logarithm- bound over all time regimes. If the underlying distribution of the data changes over the course of the run, then an upcrossing of the test statistic over these bounds, i.e., a rejection of the null hypothesis is expected. The methods are developed for a setting when change sets in gradually in an incoming stream of data. Parameter selection for the bounds are based on simulations and methodological comparison is done with respect to existing advances. The algorithms presented here can be easily adapted to an online change-detection setting. Finally, we analyse data from several athletes and benchmark the fatigue detection results with their individual feedback over the course of the run. Qualitative conclusions on the data can be made from the martingale trajectories even in the acceptance of the null hypothesis.

Keywords: sequential & online testing, biomechanical data analysis, fatigue detection, change-point detection, martingales

Adjustable Robust Optimization for Transport Planning with Uncertain Demands

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Uncertainty in demands is a prevalent issue in manufacturing and logistics. With just-in-time approaches and minimal inventory, small changes in demand create big issues in the supply chain, but especially in the planning of transportation of goods. This leads to avoidable transports, resulting in unnecessary costs and greenhouse gas emissions.

When some of the input data is uncertain, robust optimization is a method to model these uncertainties and find efficient solutions. It is well-known that applying classic robust optimization techniques leads to overly conservative decisions, which may not always be the best course of action for real-world applications. Adjustable robust optimization (ARO) relaxes this notion by introducing a second stage, where some of the decisions can be made after the uncertain data is known. Using ARO it is usually possible to achieve better results than with classic robust optimization.

We develop an ARO model for a transportation problem where the demands for materials to be transported from a source to a sink are uncertain, taking into account all necessary physical constraints, such as maximum vehicle load and 3D cargo bay packing. We apply different uncertainty sets for the demand uncertainties (e.g. budgeted cumulative uncertainty sets) and develop methods to estimate the required parameters of these uncertainty sets. We develop different heuristic solution approaches for our ARO model and evaluate its performance on toy instances and real-world data instances.

Crack detection for 3D images of concrete using cumulative sum method

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In this talk, we present an approach for crack detection in concrete images. Our method utilizes statistical techniques, including multiple hypothesis testing and the DFS algorithm,efficient and reliable results. We address challenges such as diverse concrete characteristics, image size variations, and limited training data. By incorporating statistical analysis and leveraging these algorithms, we aim to contribute to the improvement of crack detection in concrete structures.

Risk Management in Portfolio Optimization: A Multicriteria Approach

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Portfolio optimization using the Markowitz model has been a standard approach to asset allocation, aiming to find an optimal balance between risk and return. The traditional method focuses on a single objective function, however, additional objectives like solvency ratio or transaction costs, making it challenging for a practitioner to quantify preferences and importance of each objective. Therefore, in our previous work, we have transformed the Markowitz model into a multicriteria optimization problem where we optimize return and volatility among others simultaneously as individual objective function. This has lead to a significant improvement for the asset allocation in practice. Still, decision makers face challenges due to incomplete knowledge, parameter fluctuations, and uncertainty in real-world scenarios; these can significantly impact portfolio outcomes for both classical and multicriteria Markowitz. To address these issues, this research investigates how multicriteria optimization can not only enhance the decision support for portfolio optimization but also improving the risk management and analysis, improving the robustness of the investment strategies of portfolio managers.

In this talk, we explore two use cases motivated by real-world issues to illustrate the power of multicriteria optimization in portfolio risk management. The first use case involves a sensitivity analysis for parameters in the return objective function. Usually, the expected return of an asset is based on historical data or simulations. Different approaches lead to different return values and the question arises, whether small fluctuations have a significant impact on the outcome of the optimization probblem. By utilizing the well-known weight set decomposition technique from multicriteria optimization, we identify which fluctuations of parameters are irrelevant to the outcome. This allows decision makers to focus on relevant parameters and disregard those that have minimal impact. The second use case tackles the challenge of uncertain parameters in the volatility objective function. Different scenarios, such as financial crises or economic growth, with unknown probability are considered that have an impact on the volatility parameters only. To address this uncertainty in only one objective function, we present a novel multicriteria robust optimization concept that generalizes the well-known min-regret-robustness from single objective optimization. Using this new approach, a multicriteria solution algorithm can generate efficient solutions capable of performing well across all scenarios.

The results of this research showcase how multicriteria optimization can offer a powerful decision support system for portfolio optimization. This enables decision makers facing incomplete and uncertain data to more informed and robust asset allocation decisions, making it particularly relevant in dynamic and uncertain financial markets.

Generalized Dominance Cones for Ordinal Optimization

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Combinatorial optimization with ordinal objective functions models situations where the impact of an element in a solution can not be quantified, i.e., the objective functions are based on categories (like good, medium and bad) rather than cost coefficients [Schäfer et al., 2021]. Such ordinal objective functions arise, e.g., in bike routing problems with safety criteria, where streets are categorized as "safe", "intermediate" or "unsafe", which can not be easily quantified and is not additive. Let $\mathcal{C} = \{\eta_1, \dots, \eta_K\}$ be the set of ordered categories. When solving an ordinal shortest path problem, a path with a single unsafe edge is incomparable to a path with an arbitrary number of safe or intermediate edges.

Motivated by this we extend the notion of ordinal dominance. We introduce weights $\omega_i \geq 0$ and $\gamma_i \geq 0$ for $i = 1, \dots, K-1$. Thereby, ω_i represents the (maximum) number of elements of category η_i which are still strictly preferred over one element of category η_{i+1}, and for $\gamma > 0$, $1/\gamma_i$ defines the number of elements of a category η_i which are strictly worse than one element of category η_{i+1}. If $\gamma = 0$, no set of elements in category η_i is dominated by an element in category η_{i-1}. This allows to model more general dominance structures, which include classical ordinal, lexicographic and Pareto dominance as special cases.

In [Klamroth et al., 2023] it is shown that ordinal optimization problems can be represented by a vector optimization problem, which can be (linearly) transformed into a standard multi-objective optimization problem. This result transfers also to generalized ordinal optimization problems.

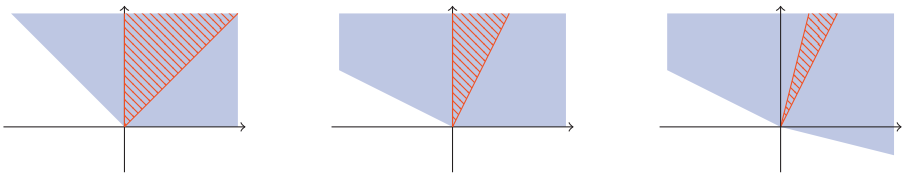

Figure 1: Generalized ordinal cones with two categories (dominance cone in blue, dual cone in red). Left: Ordinal dominance ($\omega = 1, \gamma = 0$), middle: ($\omega = 2, \gamma = 0$), right: ($\omega = 2, \gamma = \frac{1}{4}$)

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3D Microstructure Image Generation using GANs with Minkowski Functionals for Fuel Cell Electrodes[1]

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The generation of realistic 3D microstructure images is crucial for understanding and optimizing materials in various fields, including fuel cell technology [1]. In this study, we propose an approach for generating 3D microstructure images of the fuel cell electrodes using Generative Adversarial Networks (GANs) [2] with Minkowski functionals [3]. Our methodology leverages the power of GANs and integrates Minkowski functionals, specifically volume density and surface density, as key components during the training process (c.f. Figure 1). Minkowski functionals provide valuable geometric measures that capture essential characteristics of the microstructure, enabling a more accurate representation and generation of the intricate details.

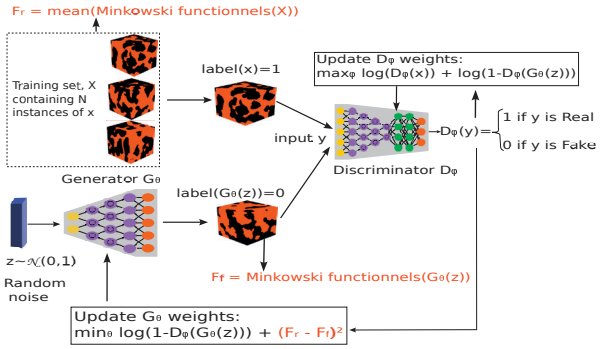

Figure 1: Overview of our proposed GAN with Minkowski functionals for 3D microstructure image generation.

During training, the Minkowski functionals are incorporated as loss functions to guide the generator's learning process. By incorporating these functionals into the GAN framework, we aim to capture the complex spatial patterns and statistical properties of the microstructures accurately.

Through experimental evaluation, we demonstrate that our approach generates realistic 3D microstructure images of the fuel cell electrodes. The generated images exhibit the desired phase distribution and capture the fine-scale details present in the real microstructures.

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Parameter Identification by Deep Learning of a Material Model for Granular Media

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Classical physical modelling with associated numerical simulation (model-based), and prognostic methods based on the analysis of large amounts of data (data-driven) are the two most common methods used for the mapping of complex physical processes. The efficient combination of these approaches has become increasingly important in recent years. Continuum mechanics in the core consists of conservation equations that can be supplemented by phenomenological material models in addition to the always necessary specification of the process conditions. The latter are an idealised image of the specific material behaviour that can be determined experimentally, empirically, and based on a wealth of expert knowledge. The more complex the material, the more difficult the calibration is. This situation forms the starting point for this work's hybrid data-driven and model-based approach for mapping a complex physical process in continuum mechanics. Specifically, we use data generated from a classical physical model by the MESHFREE simulation [1] to train a Principal Component Analysis-based neural network (PCA-NN) [2] [3] for the task of parameter identification of the material model parameters. The obtained results highlight the potential of deep-learning-based hybrid models for determining parameters, which are the key to characterising materials occurring naturally, and their use in industrial applications (e.g. the interaction of vehicles with sand).

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A Fast Surrogate Model for the Monto-Carlo Simulation of Electron-Matter Interaction

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Scanning electron microscopy using secondary electron (SE) or electron back scatter (BSE) contrast is an important and versatily analytical tool in material science, life science, semiconductors, and other fields. Synthetically generating SE and BSE images is therefore of high interest, both as a means for the validation of experimental techniques and to mass generate training data for Deep Learning.

The most common approach is the use of Monte Carlo simulation of electron-matter interaction to compute the secondary particles that propagate through the sample. The approach has the advantage of beeing based on well understood physics and is algorithmically straight forward. The primary drawback is computational cost.

We show how to train a neural network as a surrogate model for the Monte Carlo simulation. The network accepts a virtual microstructure as inputs and generates a synthetic SE and BSE images simultaneously. The most critical part of the process is the data encoding. We show that the obvious approach of encoding the microstructure as a three-dimensional array of voxels does not work. Instead, we use a combination of exteneded heightfields and normal maps.

The neural network is not capable to recreate the noise inherent to the electron imaging process and generates noise-free images instead. This can be beneficial for some applications. If the noise is required in the synthetic iamges, it can be added algorithmially as a post-processing step.

Our model requires 173 ms on average for a single image prediction on an Nvidia V100. For comparison, the original Monto-Carlo simulation requires an average of 114 min, so we achieve a speedup of 4-5 orders of magnitude. However, the original simulation code is not fully optimized and uses a single thread of an Intel Xeon Gold 6240R CPU, so our results do not allow for any quantitative performance comparison of the algorithms.

Positivity Preserving Time Integration Schemes for Balance Laws

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In the talk we will present so-called modified Patankar-Runge-Kutta (MPRK) schemes. They adapt explicit Runge-Kutta schemes in a way to ensure positivity and conservativity irrespective of the time step size. Thereby, we introduce a general definition of MPRK schemes. Additionally, we present necessary as well as sufficient conditions to derive first, second and third order accurate MPRK schemes and investigate their stability regions. The theoretical results will be confirmed by numerical experiments in which MPRK schemes are applied to solve non-stiff and stiff systems of ordinary differential equations. Furthermore, we investigate the efficiency of MPRK schemes in the context of convection-diffusion-reaction equations with source terms of production-destruction type.

MESHFREE: a way to ensure reliability of industrial simulations in fluid and continuum mechanics

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MESHFREE is a simulation tool that originates from Fraunhofer ITWM. It is designed to solve industrial and scientific problems in fluid and continuum mechanics. Its geometrical basis is a non-meshed point cloud which moves in Lagrangian sense with the velocity of the continuum. The basis of approximation is a so called moving-least-squares-approach (MLS) which provides a desired order of approximation accuracy.

Due to its design, MESHFREE is especially capable to address problems with dynamic free surfaces and phase boundaries, complex geometries and kinematics, fluid-structure interaction, and complex physics.

In order to proof the validity of a simulation result, the classical way in numerical mathematics would be to proof convergence of the simulation result upon refinement of the geometrical basis (using finer and finer geometrical resolution) and/or upon usage of higher orders of approximation. However, this way of quality-testimonial is often ignored in practical or industrial applications as it is time and resource consuming. This, indeed, is a conflict.

MESHFREE might provide a practicable solution to this conflict. On one hand, MLS allows to precisely estimate the local approximation errors and thus establish reliable quality measures of the simulation result. On the other hand, it is almost trivial to locally refine or coarsen the point cloud in order to gain particular quality targets.

In this way, MESHFREE can provide simulation results with user-requested quality. Moreover, if the user has limited computational or time resources, MESHFREE can provide the qualitatively best solution with the given resources. This widely enhances the scope of industrial applicability of simulations in general. Based on an industrial example from chemical engineering (PUR-foaming processes), quality-triggered adaptivity of MESHFREE simulations will be demonstrated.

Classification of materials using Topological Data Analysis

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Topological Data Analysis provides new approaches for interpretation of (high dimensional) data exploiting underlying structures and relationships to be used as proxies for understanding qualitative similarities and differences. Suitable vectorization of such proxies like the persistence diagram can enhance Machine Learning (ML) algorithms with an intermediate layer improving performance as well as giving interpretations of the data. Surface topography and roughness evaluation plays an important role in many problems such as friction, contact deformation or coat adhesion. Impact surface treatments can be used to improve the properties of the treated surface in the cases mentioned. Depending on the surface treatment process considered, roughness parameters listed in the ISO standards may struggle to exhibit differences between surface samples of the same material at different stages of the process. To improve existing methods and find new descriptors, we consider methods from computational topology, namely persistent homology to capture meaningful geometric features of the surface and use that to construct new surface roughness parameters better able to distinguish surface samples. Furthermore, invariants such as the persistence diagram have a rich structure which can be exploited using a plethora of different machine learning techniques. In this talk we will highlight some of the design choices and tools of TDA when introducing pipelines to understand the 2-dimensional structure of processed surfaces [1], how these compare and relate ISO standard for surface roughness and what questions/answers we are able to improve upon by combining TDA with exisiting techniques in ML pipelines.

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A variational perspective on auxetic metamaterials of checkerboard-type

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Auxetic metamaterials are pivotal for new advancements in science and engineering, as their unique ability to expand under tension and contract under compression enables diverse applications. The main result of this talk is a rigorous proof of the auxetic effective deformation behavior of elastic composites with stiff checkerboard-type heterogeneities under the assumptions of orientation preservation and non-self-interpenetration. The challenging part is the characterization of weak Sobolev limits of deformation maps whose gradients are locally close to rotations on the stiff components. To this end, we establish a new asymptotic rigidity result, showing that, in suitable scaling regimes, the attainable macroscopic deformations are affine conformal contractions, which confirms the expected negative Poisson's ratio. Our proof strategy is to tackle first an idealized model with full rigidity on the stiff tiles to acquire insight into the mechanics of the model and then transfer the findings and methodology to the model with diverging elastic constants. The latter requires, in particular, a quantitative geometric rigidity estimate for non-connected squares touching each other at their vertices and a tailored Poincaré type inequality for checkerboard structures. This is joint work with Wolf-Patrick Düll and Carolin Kreisbeck.

Random Tessellation Forests for High-dimensional Data

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Random forests are a popular class of algorithms used for regression and classification that are ensembles of randomized decision trees built from axis-aligned partitions of the feature space. One particular variant, called Mondrian random forests, was proposed to handle the online setting and is the first class of random forests for which minimax rates were obtained in arbitrary dimensions. However, the restriction to axis-aligned splits fails to capture dependencies between features, and random forest variants with oblique splits have shown improved empirical performance. By viewing the Mondrian as a special case of the stable under iteration (STIT) process in stochastic geometry, we utilize the theory of stationary random tessellations to resolve open questions about the generalization of split directions. In particular, we show that a large class of random forests with oblique splits achieve minimax rates for Lipschitz and C^2 functions and illustrate how these random tessellation forests can overcome the curse of dimensionality in high-dimensional feature space with a data-driven choice of split directions.

A stochastic gradient descent algorithm to maximize power utility of large credit portfolios under Marshall–Olkin dependence

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A vector of bankruptcy times with Marshall–Olkin multivariate exponential distribution implies a simple, yet reasonable, continuous-time model for dependent credit-risky assets with an appealing trade-off between tractability and realism. Within this framework, the maximization of expected power utility of terminal wealth requires the optimization of a concave function on a polygon, a numerical problem whose complexity grows exponentially in the number of considered assets. We demonstrate how this seemingly impractical numerical problem can be solved reliably and efficiently in order to prepare the model for practical use cases. To this end, we resort to a specifically designed factor construction for the Marshall–Olkin distribution that separates dependence parameters from idiosyncratic parameters, and we develop a tailor-made stochastic gradient descent algorithm with random constraint projections for the model's numerical implementation. Finally, we explain a new method to include transaction costs and apply the model in a real-world, high-dimensional example.

A second order level-set algorithm in topology optimisation and the topological state derivative

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In this talk we discuss first and second order methods to solve topology optimisation problems. In the first part we review the concept of the first/second topological derivative using the so-called first and second order topological state derivative associated with a partial differential equation. Usually the topological derivative of a cost functional is defined by a circular singular perturbation, however, also other types of topological perturbations can be defined. The topological state derivative and consequently the topological derivative depends on the shape/design variable and the shape of the singular perturbation chosen. For example, in dimension two the perturbation can be a ball or a circle, in dimension $n \geq 3$ a n-ball or a closed hypersurface. We show how the second order topological derivative can be used to define a second order level-set algorithm following the popular level-set algorithm of Amstutz-Andrä. In this algorithm the shape is described by a scalar level-set function ψ, the interior of the design is defined by negative values of ψ and the outside by positive values of ψ. The evolution of ψ, which is topically only driven by the first order topological derivative, is proposed to evolve by an update using second order information. Finally, we present numerical experiments for the Newton-type method for some model problems and compare it to the usual gradient-type level-set algorithm.

Recent Advances in Discrete and Robust Bilevel Optimization

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Bilevel optimization is a field of mathematical optimization in which some variables are constrained to be optimal solutions of another optimization problem. It is a rather young but very active field of research, having its game-theoretic roots in Stackelberg games introduced in the early 1930's. Over the last decades, bilevel problems have gained increasing attention both in academia and practice, due to their ability to model hierarchical decision making processes. Bilevel problems are intrinsically hard to solve – even if all objective functions and constraints are linear, all variables are continuous, and all parameters of the problem are exactly known, the problems are known to be NP-hard. However, the situation becomes more challenging if, e.g., (i) discrete variables are introduced or (ii) problems under uncertainty are considered. In this talk we will focus on these two classes of bilevel optimization problems, with a particular focus on robust bilevel optimization.

Many state-of-the-art solution approaches for bilevel optimization with integer variables make use of techniques that originate from mixed-integer programming. These techniques include branch-and-bound methods, cutting planes and, thus, branch-and-cut approaches, or problem-specific decomposition methods. In the first part of the talk, we will review bilevel-tailored approaches that exploit these mixed-integer programming techniques to solve bilevel optimization problems. We will then discuss classical ways of addressing uncertainties in bilevel optimization using stochastic or robust techniques. We will see that the sources of uncertainty in bilevel optimization can be much richer than for usual, single-level problems, since not only the problem's data can be uncertain but also the (observation of the) decisions of the two players. The talk is based on the joint research published in [1, 2, 3].

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Ontological tools and interoperability for complex materials modelling applications

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Interoperability between different data sources is becoming more and more important in applied sciences and beyond. Ontologies may be considered as a language used to express interoperability so that on the one hand people, in particular decision makers, can effectively and unambiguously communicate, and are on the other hand logically consistent so that many different digital systems may use information coming from different sources.

In this presentations, the approach followed by the Horizon2020 project VIPCOAT is highlighted. The currently developed ontological tools used to enhance the interoperability between companies aligned along a production/value chain are discussed and the mutual benefits achieved for accelerated innovation processes are sketched. VIPCOAT uses a number of materials modelling and simulation approaches to support essential steps in active protective coatings development for aeronautic applications, starting from the synthesis of novel corrosion prohibiting pigments over the optimization of a coating formulation to the behaviour of an applied coat on top of metal sheets in accelerated ageing tests. Since the output of a production step upstream the production chain forms the input of a downstream process, it is obvious that interoperability of the corresponding data streams are important to speed up such innovation processes.

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Reliable AI: Successes, Challenges, and Limitations

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Artificial intelligence is currently leading to one breakthrough after the other, both in public life with, for instance, autonomous driving and speech recognition, and in the sciences in areas such as medical imaging or molecular dynamics. However, one current major drawback is the lack of reliability of such methodologies.

In this lecture we will take a mathematical viewpoint towards this problem, showing the power of such approaches to reliability. We will first provide an introduction into this vibrant research area, focussing specifically on deep neural networks. We will then survey recent advances, in particular, concerning generalization guarantees and explainability, touching also the application of reliable AI methods to solving imaging problems and PDEs using suitable combinations of AI and model based approaches. Finally, we will discuss fundamental limitations of deep neural networks and related approaches in terms of computability, which seriously affects their reliability.

Model Order Reduction at Industrial Scale

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Model order reduction (MOR) has become an ubiquitous computational tool in many areas of the sciences in engineering. It allows to reduce the complexity of a computational problem formulated in terms of linear or nonlinear systems of algebraic or differential equations using (semi-)automatic mathematical methods. Particular situations when MOR is typically invoked are multi-query scenarios, i.e., when the same mathematical model is to be evaluated several times, and the repeated evaluation of the model is too time consuming. This is often the case, e.g., in the design phase when materials or the geometry of devices and components are changed in virtual prototyping, or in iterative schemes for optimization, optimal and feedback control as well as in uncertainty quantification and risk analysis. Recently, also the need for real-time evaluation of submodels as parts of digital twins has increased the need for efficient reduced-order models.

The last two decades have seen a tremendous development of MOR techniques. Here, we will focus on techniques for linear systems arising in various industrial contexts. We concentrate on mechanical engineering and computational mechanics on the one side and nano-electronics and electro-magnetics on the other side. In both areas, the same meta-language of systems theory for modeling the dynamics of the system can be used, focusing on the energy transport from inputs (forces, heating/cooling, applied voltages) to outputs (displacements, temperatures, currents/magnetic fields). After transformation to frequency domain, this results in an input-to-output mapping given by transfer functions. These can be approximated in several ways for obtaining reduced-order models and fast online evaluation. Here, we focus on two techniques that have evolved as gold standards: balanced truncation and rational interpolation/moment matching methods. We will describe the challenges for these approaches arising from problems at industrial scale and highlight the advances of these methodologies in recent years that now allow to apply these methods in industrial environments. We exemplify these developments for the compact modeling of machine tools and for various instances of fast verification procedures of nano-electronic devices from the semiconductor industries.

Optimization: four exciting decades of progress, and a look at what the future may hold

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Over the past four decades we have seen developments in Linear Programming (LP) and Mixed-Integer Programming (MIP) solvers that have completely transformed optimization and its applications. We will highlight some of the milestones in these developments. We will then discuss current and future trends in optimization, including the following questions: will performance improvements in LP and MIP solvers continue as they have in the past, will new kinds of solvers emerge beyond LP and MIP, and perhaps most important, can we expect optimization to play a significant role in prescriptive analytics, data science, and machine learning?

Speakers in Alphabetical Order

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