KLAIM 2025

Kaiserslautern Applied and Industrial Mathematics Days

KLAIM 2025, October 6 to 8, 2025
Book of Abstracts

Coupled Problems

KLAIM 2025 is jointly hostet by Fraunhofer Institute for Industrial Mathematics ITWM and the Department of Mathematics of RPTU University of Kaiserslautern-Landau.

Table of Contents

Welcome to KLAIM 2025 – Coupled Problems

September 2025

Dear Participants,

A cordial welcome to all of you! We are looking forward to the third edition of the Kaiserslautern Applied and Industrial Mathematics Days – KLAIM 2025 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 showcase recent results and to move forward into new research fields. In 2021, we started this new conference series, with a focus on Digital Twins, and in 2023 we continued with the conference motto Synthesis of Models and Data. This year's edition of KLAIM puts emphasis on Coupled Problems. This focus topic reflects the ever increasing complexity in today's simulation and optimization methods where different problem stages, different scales, or different physical domains and effects are connected in various ways.

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

1. **Coupling Across Scales – Multiscale Methods in the Materials Sciences**
   This track is organized in collaboration with the French-German Graduate School Mathematical image processing and synthetic microstructures for machine learning.
2. **Coupling Across Domains – Multiphysics Simulation**
3. **Co-Simulation and Control in Coupled Engineering Applications**
   This track is organized in collaboration with the ECMI Special Interest Group Math for the Digital Factory.
4. **Coupled Discrete and Bilevel Optimization Problems**
5. **Solver Coupling and High Performance Computing**

Additionally, a special session on success stories from collaboration projects with industry is organized by the European Network EU-MATHS-IN.

Mathematics in Kaiserslautern

Applied and industrial mathematics has a long tradition in Kaiserslautern. Both, the Department of Mathematics at the RPTU University Kaiserslautern-Landau and the Fraunhofer-Institute for Industrial Mathematics ITWM enjoy a high reputation for their research profiles, with the Collaborative Research Center "Symbolic Tools in Mathematics and its Application" (SFB-TRR 195), the newly established Research Training Group "Mathematics of Interdisciplinary Multiobjective Optimisation" and the NFDI project "Mathematical Research Data Initiative" as flagships (all three funded by DFG), for several research projects in the mathematics program of BMFTR and many more coordinated research projects.

Additionally, the Department of Mathematics is well known for its highly ranked study programs at the master and PhD levels, and the Fraunhofer ITWM with its around 500 employees adds numerous industrial cooperations and industry-funded research projects.

Dankeschön!

We gratefully acknowledge the support from MSO – Modelling/Simulation/Optimization, which 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 2025 a success: Stephanie Beck, Gesa Ermel, Steffen Grützner, Doris Hemmer-Kolb, Jonas Hürter, Henry Jäger, Esther Packullat, and Simone Windhagen.

Anita Schöbel

Bernd Simeon

Scientific Committee

- **Gustavo (Jesus) Angulo,** Mines Paris PSL University
- **Martin Arnold,** Universität Halle
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- **Johan Carlson,** Fraunhofer Chalmers Göteborg
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- **Anita Schöbel,** RPTU/Fraunhofer ITWM
- **Bernd Simeon,** RPTU
- **Konrad Steiner,** Fraunhofer ITWM
- **Claudia Totzeck,** Bergische Universität Wuppertal

Program

Monday, October 6th, 2025

	Auditorium	Seminar room Z03.07/08
13:30	**Welcome** Claudia Redenbach (RPTU), Anita Schöbel (Fraunhofer ITWM), Bernd Simeon (RPTU)	
13:40	**A.54 Coupling of Fields, Scales, Dimensions and Models in Forward and Backward Analyses for Crucial Applications in Engineering and the Applied Sciences (Plenary1)**[1] Wolfgang A. Wall, Institute for Computational Mechanics, Technical University of Munich, DE	
	SESSION 1 – TRACK 1 (Chair: C. Redenbach)	**SESSION 2 – TRACK 4 (Chair: T. Seidel)**
14:30	**A.55 Polynomial Matrix Inequalities in Structural Optimization (Track Plenary)**[1] Jan Zeman, Czech Technical University in Prague, CZ	**A.03 A Linear Algorithm for the Single Picker Routing Problem With Decoupling** Christian Manz, Johannes Gutenberg Universität Mainz, Framersheim, DE
		A.04 A Benders Decomposition Approach for the Single Picker Routing Problem With Scattered Storage André Hessenius, Johannes Gutenberg University, Mainz, DE
	A.07 Statistical Modeling and Generation of Inertial Ductile Fracture Surfaces Corentin Thouénon, CEA, FR	**A.41 Computation of Safe Routes to School** Michael Stiglmayr, Bergische Universität Wuppertal, DE
	A.20 Determination of the Effective Crack Resistance in Porous Materials Using a Fracture Phase-Field Model Ralf Müller, TU Darmstadt, DE	**A.45 A Mixed-Integer Linear Programming Approach for on-Demand Electric Shuttle Routing With Time Windows and Charging Constraints** Mostafa Emam, Institute of Applied Mathematics and Scientific Computing, Neubiberg, DE
16:00	Coffee break	
	SESSION 3 – TRACK 2 (Chair: C. Totzeck)	**SESSION 4 – TRACK 4 (Chair: M. Stiglmayr)**
16:30	**A.01 Multiphysical Design Optimization of Electric Machines (Track Plenary)**[1] Peter Gangl, RICAM Linz, AT	**A.30 Ordered-Median Location Problems in Intermodal Networks** Jonas Breihof, RPTU University Kaiserslautern-Landau, DE
		A.34 Solving Partial Inverse Combinatorial Problems Eva Ley, TU Braunschweig, DE
	A.06 High Performance Algorithms for Shape Optimization With Lipschitz Transformations Martin Siebenborn, Universität Koblenz, DE	**A.37 Normalizing Flow-Enhanced Variational Autoencoder With Neural ODEs for Population Modeling** Marcus Baaz, Fraunhofer-Chalmers Centre, Göteborg, SE
	A.23 Fluid Dynamical Shape Optimization for Industrial Applications Sebastian Blauth, Fraunhofer ITWM, Kaiserslautern, DE	
18:00	End of conference day 1	

1) Plenary or track plenary, 45 min. | Contributed talk, 22.5 min. (both including discussions)

Tuesday, October 7th, 2025

	Auditorium	Seminar room Z03.07/08
9:00	**A.52 On Subproblem Tradeoffs in Multiobjective Optimization (Plenary 2)**[1] Margaret M. Wiecek, School of Mathematical and Statistical Sciences, Clemson University, Clemson, US	
	SESSION 5 – TRACK 4 (Chair: J. Breihof)	**SESSION 6 – TRACK 1 (Chair: K. Steiner)**
9:50	**A.29 Integrating Sequential Optimization Problems in a Multiobjective Context** Jonas Hürter, RPTU University Kaiserslautern-Landau, DE	**A.26 Bridging Computational Time Scales in Aerosol Dynamics Prediction: Combining Monte Carlo Simulations and Neural Networks** Lukas Fuchs, Ulm University, DE
	A.46 A Hypervolume-Based Method for Multi-Objective Two-Stage Robust Optimization Problems Johannes Kager, Technische Universität München, Straubing, DE	**A.02 Efficient Multiscale Simulation of Immiscible Two-Phase Flow for Liquid Composite Molding Processes** Dominik Burr, Fraunhofer ITWM, Kaiserslautern, DE
	A.10 Parametric Linear Programming Interdiction Simon Wirschem, RPTU University Kaiserslautern-Landau, DE	**A.31 Structure-Property Relationships for Nickel-Rich Cathodes of Lithium-Ion Batteries, Using Resistor Network Simulations Based on Micro-CT Image Data** Phillip Gräfensteiner, Ulm University, DE
	A.25 A Multi-Objective Perspective on Block-Structured Integer Programs With Coupling Constraints Kathrin Klamroth, University of Wuppertal, DE	**A.12 Computing the Micromagnetic Response of a Bulk Ferromagnet by an FFT-based Method** Matti Schneider, University of Duisburg-Essen, DE
11:20	Coffee break	
	SESSION 7 – TRACK 4 (Chair: K. Klamroth)	**SESSION 8 – TRACK 2 (Chair: C. Leithäuser)**
11:40	**A.36 Inverse Robust Optimization Problems and Their Solution Using Adaptive Discretization Methods (Track Plenary)**[1] Tobias Seidel, Fraunhofer Institute for Industrial Mathematics ITWM, DE	**A.05 Unravelling the Mystery of Enhanced Open-Circuit Voltages in Nanotextured Perovskite Solar Cells** Patricio Farrell, Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Berlin, DE
		A.13 Numerical Simulation of Fluid-Structure-Acoustic Problem Motivated by Human Phonation Jan Valášek, Czech Technical University in Prague, CZ
	A.14 Reoptimization in Radiotherapy: Reducing Bilevel Problems to Single-Level Multi-Criteria Optimization Problems Mara Schubert, Fraunhofer ITWM, Kaiserslautern, DE	**A.33 Theoretical Modeling and Experimental Verification of the Electro-Thermomechanical Coupling of Shape Memory Alloy Hybrid Composites** Max Kaiser, Leibniz-Institut für Verbundwerkstoffe GmbH, Kaiserslautern, DE
	A.40 Solving Adjustable Robust Problems by Bilevel Optimization Techniques Kerstin Schneider, Fraunhofer ITWM, Kaiserslautern, DE	**A.27 Sequential Quadratic and Convex Optimisation With FEniCSx and PETSc** Paul T. Kühner, University of Luxembourg, Esch-Belval Esch-sur-Alzette, LU
13:10	Lunch break	
	SESSION 9 – TRACK 3 (Chair: B. Simeon)	**SESSION 10 – TRACK 1 (Chair: H. Andrä)**
14:30	**A.48 Computational Dynamics Towards Artificial Intelligence (Track Plenary)**[1] Johannes Gerstmayr, University of Innsbruck, AT	**A.44 Predicting the 3D Nanostructure of SOFC Anodes From 2D SEM Images Using Spatial Stochastic Modeling and CNNs** Léon Schröder, Ulm University, DE
		A.09 Two-Scale Geometric Microstructure Modeling of Wood Fiber Insulation Mats Alex Keilmann, RPTU University Kaiserslautern-Landau, DE
	A.21 Towards Fast-Response AI Models for Wheel Loader-Granular Material Interaction Based on Validated DEM-MBD Simulations Pontus Malmsköld, Fraunhofer Chalmers Centre, Gothenburg, SE	**A.39 Multiscale Approach to Super-Resolve X-Ct Data of Crushed Fayalite Slag, Using Generative Adversarial Networks** Tom Kirstein, Ulm University, Neu-Ulm, DE
	A.51 Dual-Mode Model Predictive Motion Cueing for Robot-Based Driving Simulators Tim Nicolai, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE	**A.43 Hybrid Classical–Quantum Pipeline for Crack Detection Using VQLS-Enhanced QSVMs** Akshaya Srinivasan, Fraunhofer ITWM, Kaiserslautern, DE
16:00	Coffee break	
	SESSION 11 – TRACK 3 (Chair: M. Burger)	**SESSION 12 – TRACK 5 (Chair: C. Fieker)**
16:20	**A.50 Multiscale Coupling for the Usage-Specific Simulation of Battery-Electric Vehicles** Karen Luka Schmidt, Fraunhofer ITWM, Kaiserslautern, DE	**A.22 Coupling Computational Mathematics Software: A Brief Review of Practices in SageMath and Friends (Track Plenary)**[1] Nicolas M. Thiéry, Université Paris-Saclay, Gif-sur-Yvette, FR
	A.35 Straightforward Computation of Interface-Jacobian and Coupling Sensitivities for Co-Simulation and Solver-Coupling Techniques Stefan Klimmek, TU Darmstadt, DE	
	A.17 Virtual Planning and Optimization of Factory Layouts Raad Salman, Fraunhofer-Chalmers Centre, Gothenburg, SE	**A.47 The OSCAR Computer Algebra System** Max Horn, RPTU University Kaiserslautern-Landau, DE
	A.49 Cancelled: ~~Reduced Order Models in Wheel-Rail Applications~~ ~~Diana Manvelyan-Stroot, Siemens AG, Garching bei München, DE~~	
17:50	End of conference day 2	
18:30	Conference dinner	

1) Plenary or track plenary, 45 min. | Contributed talk, 22.5 min. (both including discussions)

Wednesday, October 8th, 2025

	Auditorium	Seminar room Z03.07/08
	SESSION 13 – TRACK 5 (Chair: M. Horn)	**SESSION 14 – TRACK 1**
9:00	**A.54 Tools for High Performance Treatment of Coupled Problems (Track Plenary)**[1] Marc Alexander Schweitzer, Fraunhofer Institute for Algorithms and Scientific Computing SCAI, Sankt Augustin, DE	**Session cancelled**
	A.42 Adaptive Coupled Multiphysics Simulations With Trixi.jl Simon Candelaresi, University of Augsburg, DE	
10:10	Coffee break	
	SESSION 15 (SPECIAL TRACK)	**SESSION 16 – TRACK 5 (Chair: M. Rahn)**
10:30	**A.28 EU-MATHS-IN – Mathematics for Innovation: Success Stories and Support for European Industries** Matthias Ehrhardt, University of Wuppertal, DE	**A.08 Phase-Field Modeling of Fluid-Solid Single-Phase Flow: Solution Strategies** Cedric Riethmüller, University of Stuttgart, DE
	A.24 Costumer Segmentation in Automotive Companies Jorge Santos, LEMA – Mathematics Engineering Lab, PT	**A.38 Accelerated Permeability Prediction in Fibrous Microstructures Using Deep Learning and CFD Coupling** Stefano Cassola, Leibniz-Institut für Verbundwerkstoffe, Kaiserslautern, DE
	A.15 Cancelled: ~~**Accelerating Innovation in Circular Composite Materials Through Integration of in-Silico Design Methodologies**~~ ~~Panayiota Katsamba, University of Technology, Limassol, CY~~ **A.16** Replaced: **Evading Regulation, Entering Ecosystems: A Microscale Modelling Lens on Microplastic Fibres** Speaker: Christos Marangos, Cyprus Institute, Nikosia, CY	**A.11** New talk: **Deep Material Networks for Multi-Scale Fatigue Simulation of Fiber-Reinforced Composites** Pavan Bhat Keelanje Srinivas, Fraunhofer ITWM, Kaiserslautern, DE
11:45	**A.18 Efficient Coupling of Physics-Based Local Surrogate Models for Linear Parametric PDEs via Overlapping Domain Decomposition (Plenary 3)**[1] Marco Discacciati, Loughborough University, UK	
12:35	**Closing remarks**	
14:00	**KOMSO Meeting**	

1) Plenary or track plenary, 45 min. | Contributed talk, 22.5 min. (both including discussions)

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- Visitors have to be registered when they come to the Fraunhofer institute.
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- Photography and video recordings are prohibited.

Abstracts

Multiphysical design optimization of electric machines

Peter Gangl[1], Nepomuk Krenn[1]

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Electric machines play a major role in combatting climate change. As a consequence, the use of topology optimization methods for determining their optimal design has become increasingly popular over the past years. Beside electromagnetic performance, also thermal aspects play a more and more important role due to a desired increase in power density and a recent trend to high speed machines.

In this talk, we employ a multi-material level set algorithm based on the mathematical concept of topological derivatives to the design optimization of electric machines. More precisely, we aim at finding the optimal material distribution consisting of ferromagnetic material, air and permanent magnets in order to maximize the torque produced by the machine. We impose constraints on both the maximum temperature due to energy losses in the machine and the maximum mechanical stresses due to the centrifugal force. In addition, by imposing constraints on the magnetic fields, we aim to find designs which are insensitive with respect to demagnetization of the magnets when the machine is operated at higher input current. Moreover, we discuss the robustification of the optimization method when source current or material parameters are subject to uncertainty and an extension to a realistic drive cycle setting where multiple operating points are considered.

Efficient Multiscale Simulation of Immiscible Two-Phase Flow for Liquid Composite Molding Processes

Dominik Burr[1,2], Stefan Rief[1], Konrad Steiner[1]

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The simulation of immiscible two-phase flow is of interest in multiple applications. Traditionally it is often used in geology. But there are also industrial processes in which it could be used to get a better understanding of the process and possibly enhance it. Examples for such industrial processes are the electrolyte filling of lithium-ion batteries, transport processes in fuel cells or the production of composite materials.
In this talk, a procedure to simulate the infiltration of a fluid into a multiscale porous material that is initially filled with a second fluid is presented. The porous material in the considered example contains three distinct length scales that we denote by micro-, meso- and macroscale from the smallest to the largest. To circumvent expensive simulations on the mesoscale, we developed a generalization of a pore-morphology method to mesoscale geometries.

The simulation procedure is explained and applied to a Liquid Composite Molding (LCM) process. The LCM process is a manufacturing process of composite materials in which a thermoset polymer resin is injected into a textile stack. The textile stack consists of multiple layers of fiber mats. The fiber mats are made of woven rovings and the rovings themselves consist of hundreds of filaments. In this example the macroscale is the complete textile stack. The mesoscale consists of a section of multiple fiber mats stacked on each other and the microscale is a section of a single roving.
We start by creating representative geometries of the microscale and simulate their material parameters. To do this efficiently we use a pore-morphology method. On the mesoscale, the pore-morphology method cannot be used because the mesoscale consists of solid-free pores as well as effective porous material and the pore-morphology method only works on pore-scale geometries. To circumvent this restriction, we developed a generalization of the pore-morphology method. With this generalization, it possible to efficiently calculate the material parameters of the mesoscale. Using these the dynamic two-phase flow can be simulated on the macroscale. To do this, we implemented an IMplicit Pressure Explicit Saturation (IMPES) method with a finite volume discretization and an adaptive timestep criterion. This solver is verified for pressure drop dominated and capillary pressure dominated flows and can handle compressible fluid phases as well as discontinuous material parameters.
Using this multiscale procedure, it is possible to efficiently calculate the material parameters of the textile stack and set up a dynamic macroscale simulation of the LCM process.

A Linear Algorithm for the Single Picker Routing Problem with Decoupling

Christian Manz[1], André Hessenius[2], Stefan Irnich[3]

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The standard single-picker routing problem (SPRP) seeks a cost-minimal tour to collect a set of articles in a given warehouse layout. We present a new solution for the decoupling extension. The single-picker routing problem with decoupling (SPRP-D) also seeks a cost-minimal tour in a warehouse where each article is located once, but additionally the picker has the opportunity to decouple from the cart and collect a small set of items by hand. It is a classical result that Ratliff and Rosenthal solve the SPRP in linear time by searching a shortest path in a state space that models the warehouse. We extend this state space to model the decoupling of picker and cart. Thus we provide the first polynomial and especially linear runtime algorithm to solve the SPRP-D. In related work, the setting is restrictive. Picker and cart can only decouple in certain locations and the speed ratio between cart and picker is bounded. We also extend the decoupling possibilities and allow a larger variety in picker moves. Computational experiments show that our approach is several orders of magnitude faster than the few other approaches porposed in literature. Additionally we evaluate our other extensions in terms of runtime and additional cost savings.

A Benders Decomposition Approach for the Single Picker Routing Problem with Scattered Storage

André Hessenius[1], Christian Manz[2], Stefan Irnich[3]

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We present a new solution approach for the single-picker routing problem with scattered storage (SPRP-SS) for order picking in warehouses. Heßler and Irnich showed how to construct an extension to the Ratliff Rosenthal state space that takes care of the scattered storage extension. Based on this extended state space we propose a mixed-integer program (MIP) that splits the simultaneous decision of pick positions for requested articles and determination of the shortest route that collects all articles. This novel MIP offers an ideal starting point for a Benders Decomposition approach by first suggesting a set of positions to visit in the master and then computing the cost of this suggestion in the subproblem. To accelerate the convergence of Benders decomposition, this paper closely analyzes the feedback of the subproblem (optimality cuts). We present the most popular cuts in literature (Magnanti Wong cuts), analyze what defines a strong cut and propose a novel subproblem to generate *Core-Maximal Cuts* which lead to faster runtime than Magnanti Wong cuts. This approach is not only applicable for single-block parallel-aisle warehouses but also generalizeable: the solution procedure can be applied to each extension (e.g. different warehouse layout, other start and endpoints, ...) that can be modeled using a state space. Moreover, we provide *Core-Maximal Cuts* in a general form so they can be applied to any Benders subproblem.

Unravelling the mystery of enhanced open-circuit voltages in nanotextured perovskite solar cells

Dilara Abdel,[a] Jacob Relle,[bc] Thomas Kirchartz,[de] Patrick Jaap,[f] Jürgen Fuhrmann,[f] Sven Burger,[cg] Christiane Becker,[bh] Klaus Jäger[bc] and Patricio Farrell[a]

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[b] *Dept. Optics for Solar Energy, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany.*
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[d] *IMD-3 Photovoltaics, Forschungszentrum Jülich GmbH, Jülich, Germany.*
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[f] *Numerical Mathematics and Scientific Computing, Weierstrass Institute for Applied Analysis and Stochastics (WIAS), Berlin, Germany.*
[g] *JCMwave GmbH, Berlin, Germany.*
[h] *Hochschule für Technik und Wirtschaft Berlin, Berlin, Germany.*

Perovskite solar cells have reached power conversion efficiencies that rival those of established silicon photovoltaic technologies. Nanotextures in perovskite solar cells optimise light trapping and scattering, thereby improving optical absorption. In addition, nanotextures have been experimentally shown to enhance electronic performance, in particular, by increasing the open-circuit voltage V_{OC} – a phenomenon that, until now, has remained not fully understood. This study investigates the underlying reasons by combining multi-dimensional optical and charge-transport simulations for a single-junction perovskite solar cell. Our results reveal that the increased open-circuit voltage is not driven by optical effects but by the textured geometry itself. For voltages near V_{OC}, texturing one of the absorber/transport layer interfaces increases the imbalance between electron and hole densities in the absorber, thereby reducing Shockley-Read-Hall (SRH) recombination, which is the dominant loss mechanism in this study. While idealised solar cells benefit unconditionally from increasing texture height, in realistic cells there is an optimal texture height which maximizes the power conversion efficiency. These findings provide new insights into the opto-electronic advantages of texturing and offer guidance for the design of next-generation textured perovskite-based solar cells, light emitting diodes, and photodetectors.

High Performance Algorithms for Shape Optimization with Lipschitz Transformations

Martin Siebenborn[1], José Pinzon[2]

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Shape optimization constrained to partial differential equations is a vivid discipline in the field of optimal control with a variety of applications. This ranges from the optimization of exterior contours of solid bodies, e.g. drag reduction of an aerodynamic specimen, to the estimation of interior interfaces, which distinguish discrete, spatially distributed parameters or material properties. In this talk we present our advances in the development of optimization algorithms, that are focused on efficiency and scalability as well as on robustness with respect to geometric deformations. These questions are tightly coupled with the definition of an appropriate space of admissible shapes and the corresponding space of deformations. We comment on the computational performance of shape optimization algorithms which approximate Lipschitz transformations in two different ways. A first approach, which approximates the appropriate

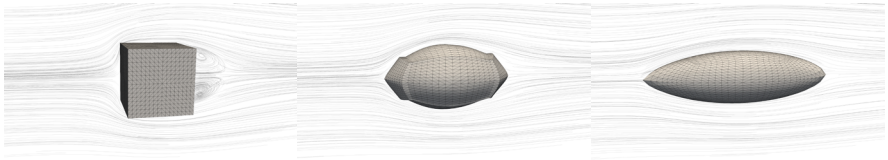

Figure 1: Inital (left) and optimized (right) obstacle in a stationary incompressible Navier-Stokes flow.

space by a p-Laplace relaxation, is computationally compared with a second one, where an alternating direction method of multipliers (ADMM) is applied. In order to achieve algorithmic scalability up to extreme scales, we apply geometric multigrid preconditioners to the numerical solvers. A particular focus is on the deformation of the underlying hierarchical grid structure during the optimization and how it influences the solver performance. The achieved results are demonstrated for classical benchmark problems in fluid-dynamic shape optimization. For this setup to be meaningful and exclude trivial solutions, the incorporation of additional, geometric constraints is essential. We discuss how this can be achieved in a scalable HPC framework. In the setting of Lipschitz transformations we present a second order approach, which follows the nonlinear solution manifold of the geometric constraints. A particular focus here is on the estimation of computational effort and scalability when, due to the faster convergence of the second order descent method, trading a large number of elliptic PDE solves for a significantly reduced number of linearized Navier-Stokes solves.

Statistical modeling and generation of inertial ductile fracture surfaces

Corentin Thouénon[1,2,3], Alizée Dubois[1,2], Jacques Besson[3], François Willot[4]

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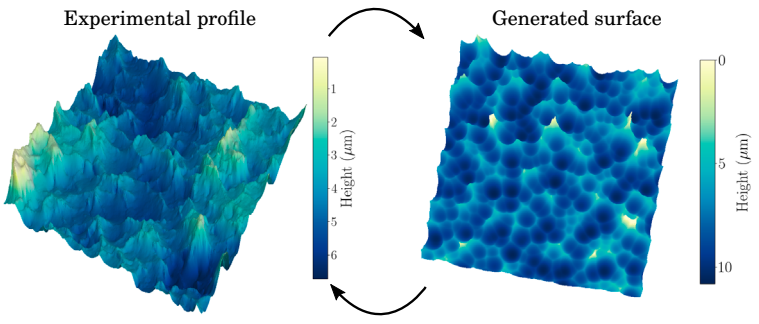
Spalling is a fundamental damage phenomenon observed in materials under dynamic loading. It occurs when two release waves interact after shock reflections, generating a high-stress region that drives the nucleation, growth, and coalescence of voids in ductile materials. By adjusting strain rates and shock pressures —through different shock generation methods such as mechanical impact or laser shock— it is possible to modify fracture properties. A key parameter in inertial damage models is the initial outer radius of the hollow sphere representing a void. This parameter governs the overall behavior of these models by influencing, for instance, the void growth rate and, consequently, the macroscopic response of the material. However, accurately determining this parameter experimentally remains a major challenge.

This study combines shock experiments, stereo-imaging-based reconstructions and image segmentation of spall surfaces to estimate the pore radius distributions and the spatial arrangement of nucleation centers. The analysis reveals a spatially random (Poisson) nucleation pattern, supporting the assumption of stochastic nucleation. This assumption is then used to build a generative model of spall surfaces based on Boolean functions. The model is introduced in three stages of increasing complexity and systematically compared to the experimental surface. This comparison highlights the need to incorporate macroscopic surface correlations to accurately reproduce the height fluctuation statistics at the scale of the dimples.



Phase-field modeling of fluid-solid single-phase flow: Solution strategies

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In this talk, we introduce a coupled Cahn-Hilliard Navier-Stokes model of fluid-solid single-phase flow. We briefly investigate the thermodynamic consistency making use of an energy-dissipation inequality and derive a thermodynamically consistent discretization based on a semi-implicit time-discretization. The energy-dissipative behavior is illustrated in numerical experiments.

Following the discretization, a key focus of this talk lies on solving the large, sparse and ill-conditioned linear systems inherent to Newton's method applied to the resulting nonlinear problem. Here, we focus on the partitioned setting where subproblems for the phase-field evolution and the fluid flow are solved alternately. We establish solution strategies building on problem-adapted preconditioners and assess their efficiency and robustness in further numerical experiments.

Lastly, we discuss approaches to make the generated data available for subsequent use. This is achieved in accordance with the FAIR and Open Data practices implemented by the Mathematical Research Data Initiative (MaRDI), such as model documentation and data storage.

Two-scale Geometric Microstructure Modeling of Wood Fiber Insulation Mats

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For the insulation of buildings, wood fiber mats are currently of high interest as they are recyclable and made from a renewable resource. However, their performance does not yet reach the one of conventional materials. The microstructure of the mats is a key influencing factor for their thermal insulation. We therefore aim to optimize the microstructure by creating digital twins for thermal conductivity simulations.

The fiber mats are highly porous (3 % - 10 % solid volume fraction) and consist of single fibers and fiber bundles, which may vary strongly in size and orientation. Hence, we construct an efficient stochastic model to generate realizations that are large enough to represent the variability in the data. Moreover, the contact between fibers is highly relevant for thermal conductivity in the solid phase. This requires us to model the interaction between fibers at a high resolution.

We satisfy the conflicting needs of resolution and representativity by two-scale geometric modeling: For large representative volume elements (RVEs), we fit a coarser model – a Boolean model with cuboids mimicking the fibers and fiber bundles. On a finer scale, we extend the Altendorf-Jeulin model for systems of curved fibers so that we can efficiently calculate and increase the number of inter-fiber contacts. Finally, the results of thermal simulations on the fine- and coarse-scale models will be coupled, thus allowing for accurate and efficient thermal simulations.

Parametric Linear Programming Interdiction

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We study the parametric linear programming interdiction problem, where an interdictor seeks to deteriorate the optimal objective value of a linear program using limited resources (budget). Interdiction problems are a special case of bilevel optimization problems where the inner problem's objective is diametrically opposed to the outer problem's objective. This problem class is well-suited for detecting weak spots and to measure a system's robustness against worst-case influences. While most existing work on interdiction focuses on networks, we consider a more general setting where the follower solves an arbitrary linear program. In our formulation, the leader's budget acts as a parameter, allowing us to examine how the impact of interdiction evolves as this budget varies. This parametric perspective reflects a natural robustness analysis: any fixed budget represents an arbitrary threat level, whereas understanding the problem across a range of budgets offers deeper insight into the system's vulnerability and stability. That is why closely related problems are also referred to as worst case linear optimization problems under polyhedral uncertainty.

We show that the nonparametric version of this can be reformulated as a bilinear program, a well-studied class in the literature and which is known to be NP-hard. The computational complexity also carries over to our nonparametric sub-problem. Besides discussing the structure, we propose an exact procedure closely related to the dichotomic search algorithm in biobjective optimization. The algorithm computes the parametric curve of the LP interdiction's objective value. Our work enables the application of parametric worst-case analysis to the wide class of linear models, which holds potential applications in robustness, security, and adversarial optimization.

Deep Material Networks for Multi-Scale Fatigue Simulation of Fiber-Reinforced Composites

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Fiber-reinforced composites are a promising material option in the design of lightweight components with improved resilience towards fatigue damage. For modeling these materials on the component-scale, incorporating of microstructural descriptors, such as the distribution of fiber orientations and fiber volume content, is essential to ensure accurate simulation results.

In a classical multi-scale simulation framework for high-cycle fatigue, see Magino et.al. [1], an effective material behavior on the component-scale is derived by model-order-reduction (MOR). For the identification of the order-reduced model, a set of loadcases on representative, micro-resolved fiber structures are pre-computed using an FFT-based solver. Based on the fiber lengths, large representative volume elements are required, worsening computational runtime and resource requirements on the micro-scale. Moreover, while attained simulation results on the component-scale coincide well with experiments, repeated simulations, as they are for instance required in topology optimization problems, remain costly in real-life applications.

To significantly improve runtimes for both micro-scale and component-scale simulations in the online-phase, a deep material network (DMN) initially conceived by Liu et al. [2] and improved by Gajek et al. [3] is proposed for the high-cycle fatigue of long-fiber-reinforced composites. The DMN aims to fit the simulations at the microscale into a material network built with laminate mechanistic building blocks, using just linear elastic training data. Subsequently, the nonlinear high cycle fatigue damage model is solved on this DMN topology for the applied boundary conditions, thus extrapolating to get in-elastic responses.

In our presentation, an overview of the DMN construction is given and attained results for test structures and a real-life component are compared to the classical MOR approach. Moreover, examples for the improved extrapolation properties of the DMN compared to the MOR approach for increasing load amplitudes are presented.

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Computing the micromagnetic response of a bulk ferromagnet by an FFT-based method

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Micromagnetism is concerned with the evolution of the magnetisation field, taking into account magnetostatic, self-interaction and magnetic anisotropy effects (at least). From a physical point of view, different time and spatial scales interact and emerge, determining the effective behavior of such a ferromagnet. To compute the response, dedicated numerical strategies are imperative.

In the talk at hand, we discuss an implicit FFT-based method which permits to resolve such micromagnetic problems on polycrystalline domains with an insulation condition on the grain boundaries.

This talk reports on joint work with M. Vorwerk and J. Schröder, both from University of Duisburg-Essen, Institute of Mechanics.

Numerical Simulation of Fluid-Structure-Acoustic Problem Motivated by Human Phonation

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Abstract

This contribution deals with the mathematical and numerical model of very complex process represented by human phonation. It involves interaction of three different physical fields – the deformation of the vocal folds (elastic body), the complex fluid flow and the acoustics together with their mutual couplings, usually referred as the fluid-structure-acoustic interaction (FSAI), see [1]. Further, mutual contact of both vocal folds regularly appears during healthy phonation increasing the difficulty of the considered problem.

The coupling strategy with regard to their different importance will be discussed. For the case of normal speech the FSAI problem will be approximated as FSI problem with forward-coupled aeroacoustic problem. The two-dimensional FSI problem is modelled with the aid of linear elastic problem coupled to the incompressible Navier-Stokes equations in the arbitrary Lagrangian-Eulerian form. The contact treatment suitable for the chosen finite element framework is briefly introduced, see [3].

Further, the aeroacoustic problem is introduced. Two different mathematical descriptions – the Lighthill acoustic analogy and the Aeroacoustic Wave Equation, are given and used, see [2]. In the end, the parameter sensitivity study is shown and the resulting frequency spectra for phonation of vowel [u:] are presented.

Keywords: fluid-structure-acoustic interaction, human phonation, Navier-Stokes equations, finite element method, aeroacoustics.

Acknowledgment

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Reoptimization in Radiotherapy: Reducing Bilevel Problems to Single-Level Multi-Criteria Optimization Problems

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Reoptimization is a critical task for many applications that require fine-tuning an already optimized solution. Starting from an initially optimal solution, new criteria emerge that must also be optimized, subject to the constraint that the updated solution remains close to the original in terms of the initial objectives.

A prime example is radiotherapy planning, where the primary goal is to deliver a high dose to the tumor while sparing surrounding healthy tissue. Advances in physics and medicine continuously introduce new factors that influence treatment outcomes. Examples include the linear energy transfer (LET) in proton therapy, which affects biological effectiveness, or machine learning-based risk models that predict patient-specific risks, such as radiation-induced pneumonitis. Initially, these factors are insufficiently studied to determine acceptable trade-offs with established dose objectives. However, incorporating them into treatment planning while preserving the optimal dose distribution has the potential to improve outcomes for patients while ensuring safety. Thus, reoptimizing dose-optimal treatment plans to account for such emerging factors becomes essential.

Radiotherapy planning presents an additional challenge: achieving sufficient tumor irradiation and sparing healthy tissue are inherently conflicting objectives. Multi-criteria optimization (MCO) is commonly used to generate a set of Pareto optimal compromises between these objectives, enabling treatment planners to select the most appropriate plan for each patient. However, calculating infinitely many plans is infeasible. Instead, a representative set is typically used, with interpolation enabling navigation along the approximated Pareto front. In reoptimization scenarios, this approach fails. It is unclear how well the reoptimized plans represent the entire set or whether interpolation remains valid between them. To address this, we reformulate the reoptimization problem as a bilevel optimization problem with specific structural properties. Exploiting these properties, we reduce the bilevel problem to a single-level MCO problem by adjusting the order relation. Finally, we demonstrate how this reformulation can be practically implemented by approximating the resulting ordering cone. This approximation further enables treatment planners to regulate the tolerable relative trade-offs, helping them prioritize which plans are of interest.

Accelerating innovation in circular composite materials through integration of in-silico design methodologies

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Designing the next generation of circular materials requires a comprehensive understanding of their mechanical performance. Here, we present a computational framework for the in-silico design and optimization of AgReCOMPOSITES—sustainable, circular materials derived from recycled plastic and biochar produced from agricultural and livestock waste. This framework combines hierarchical homogenization and Finite Element Methods with experimental data to predict the mechanical performance of biochar-polymer composites, enabling the optimization of mixing ratios and geometrical configurations for superior functionality. A key focus is on the random distribution of the ellipsoidal nanoparticle reinforcements—which significantly influences the mechanical response of the composite material. In this work we developed an inverse numerical homogenization model that predicts the inclusions properties with excellent agreement to experimental data. We extend these methodologies to AgReCOMPOSITES, showcasing the potential and challenges of the computational inverse homogenization methodology in transforming sustainable, circular materials design.

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Evading Regulation, Entering Ecosystems: A Microscale Modelling Lens on Microplastic Fibres

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Projected to reach 3.1 gigatonnes by 2050, microplastic particles (<5mm) are now recognized as pervasive stressors across Earth system compartments—from oceans and freshwater systems to soils and the atmosphere—threatening aquatic life, biodiversity, and human health through their persistence, wide distribution, and toxic bioaccumulation.

Among the diverse forms of microplastics, a critically understudied form of emerging concern is that of microplastic fibres, for short microfibres. Derived primarily from synthetic textiles, they evade current microplastic regulations. Their anisotropic, filamentous morphology poses major challenges for modelling their environmental fate, transport, and degradation, leaving a critical gap in both mechanistic understanding and large-scale predictive frameworks.

Here we present our research under the MICROFIBRES Excellence Hub, which pioneers a novel bottom-up modelling approach to investigate the pollutant release dynamics of degrading microfibres in environmental contexts. We demonstrate how advances in modelling of active colloidal filaments (Slender Phoretic Filaments) can be leveraged in the context of degrading microfibres, by viewing the latter as diffusive filaments, ie chemically active bodies that release solutes to their surrounding environment via surface fluxes. By integrating microscale mathematical modelling, multi-physics simulations, and experimental input from microcosms replicating environmental stressors (UV exposure, acidity, microbial colonization), MICROFIBRES aims to decode the coupled chemo-elasto-hydro-bio interactions that drive pollutant release from fibres in aquatic, soil/sediment, and organismal settings.

Virtual planning and optimization of factory layouts

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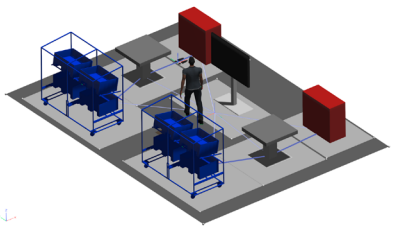
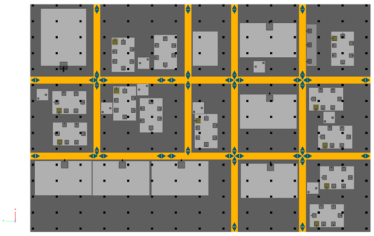
The planning of factory layouts is a complex process which involves stakeholders from diverse parts of the company organization, such as manufacturing engineers, process engineers, logistics managers, operators, ergonomics experts to name a few. These stakeholders must come to a consensus about how to balance conflicting constraints and requirements including area utilization, process efficiency, worker safety and ergonomics, and logistics efficiency. The process typically lacks digital decision support tools for even a subset of the requirements and involves many iterations between the stakeholders.

We present a digital framework where the geometric constraints for the factory layout can be formulated, visualized, and evaluated as well as a grid-based approximation approach for optimizing the placement of free resources. The optimization algorithm is centered around an efficient branch-and-bound scheme which can be used to quickly generate feasible solutions for subsequent local search heuristics or directly find the grid-optimal solution with regards to a simplified objective function. In contrast to many other examples of Facility Layout Planning problems, our problem formulation allows the resources to be modelled as arbitrary simple polygon unions and the overlapping rules are easily extensible. We give two examples of planning scenarios — manual assembly line layout planning and block-level layout planning — where the optimization algorithm can be used in conjunction with other application-specific requirements and objectives such as collision-free walking and logistics flow.



(a) Example of an assembly station layout planning scenario.



(b) Example of a factory block layout planning scenario.

Figure 1: Illustrations of layout planning scenarios.

Efficient coupling of physics-based local surrogate models for linear parametric PDEs via overlapping domain decomposition

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Simulation and control of engineering systems commonly involve multiple queries to complex, computationally-demanding solvers. Model order reduction techniques provide an established methodology for the solution of such problems, but their computational cost still constitutes a bottleneck for practical problems involving many parameters, as it is often the case in the context of multi-physics phenomena.

In this talk, a recent approach to reduce the cost of constructing surrogate models for boundary value problems governed by linear parametric PDEs will be presented [1,2]. The methodology relies on a domain decomposition (DD) rationale, where local surrogate models are computed in the offline phase using proper generalized decomposition (PGD), and then coupled via overlapping DD methods in the online phase of the algorithm.

The technique can effectively handle single- and multi-physics problems such as the Stokes-Darcy problem, for which we will discuss the suitability of an overlapping DD approach in a model-order reduction context [3,4].

Numerical results to assess the accuracy, robustness and efficiency of the proposed methodology will be presented.

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DistributedWorkflows.jl – A Julia Interface to a Task-based Workflow Management System

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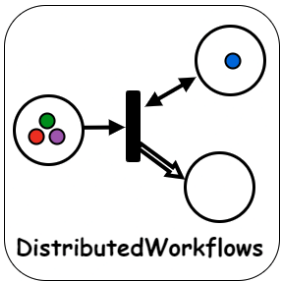

Over the last few years, Julia has gained increasing attention in the high-performance computing (HPC) community. In parallel, Julia developers have introduced packages that make HPC tools more approachable for domain scientists. This is largely due to Julia's performance-driven and user-friendly design. `DistributedWorkflows.jl` adds to this growing ecosystem of useful HPC packages.

In this talk, I will present `DistributedWorkflows.jl`, a Julia interface to a task-based workflow management system that enables users to define domain-specific workflows as high-level Petri nets, with the runtime handling task scheduling. The underlying workflow manager automatically manages application runs with dynamic scheduling, built-in distributed memory transfer, and distributed task execution.

A notable feature of `DistributedWorkflows.jl` is its independence from serialization format, making it flexible and compatible with all serializer formats supported by Julia. The primary goal is to simplify writing parallel distributed applications and empower both HPC experts and domain scientists to deploy their workflows directly from within the Julia environment.

At present, users can test and debug their workflow and application deployment locally before launching it on expensive cluster resources via SLURM or other cluster managers.

Finally, I will share a roadmap of upcoming features and improvements in distributed computing. Installation is straightforward, and a step-by-step guide is available on GitHub. This framework enables scalable automated deployment of distributed applications, allowing researchers to solve problems previously considered computationally infeasible.

Determination of the Effective Crack Resistance in Porous Materials Using a Fracture Phase-Field Model

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This work investigates the simulation-based determination of the effective fracture resistance of porous materials, taking into account both linear and non-linear material behavior. Following the approach of Hossain et al. [1], we conduct numerical experiments to identify effective crack resistance as a material parameter. Displacement boundary conditions corresponding to a steadily propagating macroscopic crack are applied to a representative microstructure. At the microscale, crack growth is simulated without prior assumptions regarding crack paths, continuity of propagation, or other features. The maximum value of the macroscopically acting J-integral defines the driving force required to advance the crack by a macroscopic length increment without arrest, which we refer to as the effective crack resistance.

To simulate crack evolution in the microstructure without predefined growth assumptions, we employ a phase-field model. Phase-field models are particularly well suited for this purpose, as they introduce a regularized approximation of cracks and an internal length scale.

In contrast to our previous work on this topic, we additionally consider non-linear material behavior using a Ramberg–Osgood-type formulation. We study the effect of the material law on the effective fracture toughness as defined in [1]. Our findings indicate that a material model allowing greater energy dissipation prior to fracture serves as a more reliable indicator of effective fracture toughness in porous materials than high tensile strength alone.

Moreover, we observe that crack re-nucleation acts as a toughness-determining failure mechanism in porous media. We investigate the influence of various parameters on the characteristic length at which cracks re-nucleate and find a strong correlation with the internal length scale of the phase-field model. Finally, we analyze the effect of pore shape and spacing in simplified porous structures, demonstrating their significant impact on the effective crack resistance and thus offering insights into failure mechanisms in porous systems.

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Towards Fast-Response AI Models for Wheel Loader–Granular Material Interaction Based on Validated DEM-MBD Simulations

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Abstract

Understanding the interaction between a wheel loader bucket and granular material is essential for optimizing performance and energy efficiency in machine design. While high-fidelity simulations based on co-simulation between the Discrete Element Method (DEM) and Multibody Dynamics (MBD) can accurately capture this interaction, their computational cost remains a limitation for certain applications such as real-time simulations or large-scale virtual testing.

Building on a previously validated coupled DEM-MBD simulation framework—supported by experimental data including point cloud tracking and onboard machine measurements—we explore a novel machine learning approach to significantly accelerate force-response prediction. In this method, the bucket geometry and motion are still resolved, but the granular material is represented using a 2D or 3D grid structure, where the interaction between the bucket and the grid cells is modeled as a modular spring-damper unit. The coefficients of these substructures are trained using machine learning techniques to reproduce force responses observed in DEM simulations.

To further enhance response realism, a trained noise model is incorporated to replicate the characteristic variability and observed in both physical experiments and high-fidelity simulations. This ongoing work supports the development of hybrid, data-driven surrogate models that retain physical interpretability and are compatible with multi-body dynamics (MBD) models, while significantly improving computational efficiency. It also outlines the next steps toward integration into virtual design and control environments.

Coupling computational mathematics software: a brief review of practices in SageMath and friends

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In many areas of mathematics, the exploration of new theories and the discovery, evaluation, or refutation of new conjectures is nowadays heavily supported by the power of machine computing; the latter indeed enables manipulating complex examples and processing large datasets in the search for regularities and counter examples. In certain cases, theorems have even been proved by reductions to brute force testing on a finite amount of data.

More often than not, computations require to couple new bespoke code specific to the theory at hand together with many other preexisting tools. For instance, a computation in algebraic combinatorics, the field of the author, typically involves a combination of combinatorics, exact arithmetic, linear algebra, (semi)group theory and (multivariate) polynomials if not formal power series.

To fulfill this need, the mathematical community has developed over the last two decades general purpose open source computational mathematics systems like SageMath and now OSCAR. These build on many specialized systems, the development of some of which like Antic, GAP, Maxima, Polymake, PARI/GP, or Singular required the dedicated work of dozens of researchers for up to four decades. SageMath, for example, combines together more than a hundred systems and databases, adding over a million lines of code, and offers thousands of mathematical objects to compute with. A major challenge in the design and implementation of such a system is therefore composability.

To setup the stage, the talk will begin with a brief introduction to the SageMath system, its features, and components. We will then delve into concrete examples, to review some of the challenges that arise at different scales – e.g. from SIMD parallelism to remote procedure calls – and strategies that have been used or explored for composing computational mathematical software.

Fluid Dynamical Shape Optimization for Industrial Applications

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The design optimization of flow components for industrial applications is inherently complex. Techniques from PDE constrained shape optimization, which do not rely on a-priori parametrization of the domain, can facilitate the solution of such problems. The mathematical research carried out in recent years, which is primarily focused on the advancement of solution algorithms and mesh deformations, has helped these methods to mature. Moreover, improvements in additive manufacturing allow the manufacturability of completely novel designs and facilitate the application of shape optimization to industrial applications.

In this talk, we will present our shape optimization approach for fluid dynamical applications. This includes our open-source software package cashocs, which automates the solution of shape optimization problems, as well as the methods implemented within the software. As applications, we consider the optimization of structured packings for distillation columns, the optimization of fiber patterns for industrial spinning processes, as well as the optimization of (electro-) chemical reactors. For all of these applications, shape optimization provides novel design ideas and helps to leverage previously undiscovered potentials.

Costumer Segmentation in Automotive Companies

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LEMA, the Mathematical Engineering Laboratory, has been working with the NORS holding group since 2021 in the segmentation of its companies' customers. Among the various segmentation algorithms implemented for different companies, the RFM approach stands out. This approach is based on the use of three variables: (R)ecency, (F)requency, and (M)onetization. These variables describe the behavior of customers regarding their interaction with the company. Recency defines the number of days since the customer last interacted with the company. Frequency and Monetization defines, in a given time period, respectively, the number of interactions the customer has with the company, and the amount spent by the customer.

The RFM approach combines these three variables with the aim of segmenting the customer's. This combination can take several forms. Examples are:

1. RFM variables can be divided into intervals (usually 5). A given customer is segmented according to the intervals to which he belongs. For example, if the customer is in intervals 2, 4 and 5 for, respectively, the Recency, the Frequency, and the Monetization, his situation [245] can be converted into a given segment according to a previously defined table with the various combinations of values.

2. The variables can be combined according to a formula that reflects the importance that the company attributes to each of them. A weighted average of the values of the intervals $\alpha_1 R + \alpha_2 F + \alpha_3 M$ can be obtained, thus obtaining a score that can correspond to a given level (segment).

The levels and combinations for obtaining the different segments are arranged in close collaboration with the company's business managers.

The segmentations obtained with these methods were analyzed by the managers and, in some cases, compared with the segmentations already used by the company. In both cases, the results exceeded initial expectations and these algorithms became commonly used by the companies. In some cases, validation of the Pareto principle demonstrated the dependence of some companies on a very small number of customers, an undesirable situation that merited reflection by the managers.

The inclusion of additional variables in the RFM model that may reflect the financial health, geographical location or even the weight of each business area has been tested in some companies with considerable success.

Other approaches in the area of machine learning, namely clustering algorithms, have also been used to achieve a solution less dependent on the business manager. Despite the satisfactory results and the new insights, they revealed some limitations and the importance of those managers in this type of problem.

A Multi-Objective Perspective on Block-Structured Integer Programs with Coupling Constraints

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We seek to solve block-structured integer programs with a single coupling constraint by interpreting the coupling constraint as a second objective. This reformulation results in an additively-separable bi-objective optimization problem with a solution set which contains the optimal solution to the original problem. The resulting bi-objective problem is harder to solve. We therefore propose ways of directing the search for nondominated solutions to only require solutions mapping to a predefined region of interest. This approach allows us to use decomposition methods while also providing the decision maker with a set of alternative 'interesting' solutions.

Bridging Computational Time Scales in Aerosol Dynamics Prediction: Combining Monte Carlo Simulations and Neural Networks

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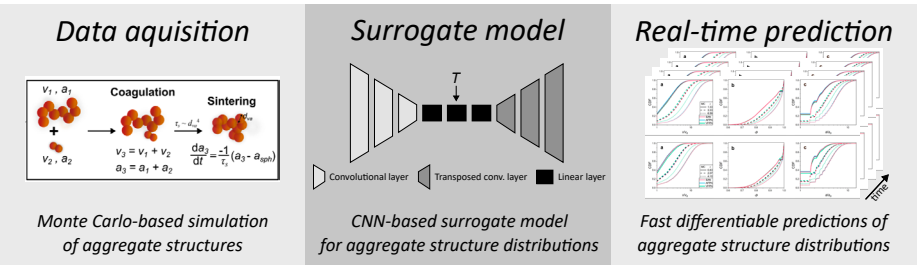
Coupled problems across multiple computational time scales are a major challenge in modern materials science, where the prediction of aggregation dynamics is fundamental for controlling synthesis processes. This talk addresses a key bottleneck: Often, computational times of models for aggregation dynamics exceed the actual time scales of real aggregation processes, making them unsuitable for real-time process control.

We present a novel approach that couples bivariate Monte Carlo (MC) simulations of aerosol dynamics with convolutional neural network (CNN)-based surrogate models, achieving a 15,000-fold acceleration in computational speed. The MC framework models particle coagulation and sintering dynamics in high-temperature gas phase synthesis through population balance equations, tracking both particle volume and surface area evolution over time. Based on data simulated with the MC framework, a CNN surrogate with an autoencoder architecture is trained to predict bivariate histograms of particle sphericity and volume distributions as a function of arc reactor temperature and time.

The proposed methodology transforms intensive simulations, requiring 1,883 seconds for full time-series prediction, into real-time-capable predictions completed in just 0.118 seconds. The surrogate model's CNN structure and low computational costs enable efficient reactor temperature optimization to achieve desired aggregate descriptor distributions. This approach makes model-based control viable for applications such as arc discharge, spark discharge, flame spray pyrolysis, and hot-wall reactor processes.



Sequential Quadratic and Convex Optimisation with FEniCSx and PETSc

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Efficient solution of large-scale PDE-constrained optimisation problems demands both problem-specific algorithms and highly performant implementations. Balancing these requirements remains a significant challenge across many application domains.

We present simple, customisable implementations of Sequential Quadratic Programming (SQP) and Sequential Convex Programming (SCP) methods [1] that facilitate rapid prototyping while leveraging the efficiency of established open-source libraries. In particular we focus on the famous separable approximations CONLIN [2], the Method of Moving Asymptotes (MMA) [3], and their variants.

In our framework, `FEniCSx` [4] is employed for the assembly of finite-element discretisations, and the custom optimisation routines are built atop those provided by `PETSc` [5]. All code is freely available as part of the `dolfiny` project [6]. To illustrate the capabilities and verify the accuracy of our approach, we consider benchmark PDE-constrained optimisation problems and compare convergence behaviour and computational performance. We further demonstrate applications in structural mechanics, including both shape and topology optimisation.

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EU-MATHS-IN -- MATHEMATICS FOR INNOVATION: SUCCESS STORIES & SUPPORT FOR EUROPEAN INDUSTRIES

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1. **M. Ehrhardt, University of Wuppertal, Germany, "EU-MATHS-IN OpenDesk: a European One-Stop Shop for Researchers and Entrepreneurs" (keynote)**

Abstract: Industrial mathematics plays a vital role in driving innovation and competitiveness across sectors, offering powerful tools to solve complex industrial challenges. The EU-MATHS-IN network, comprising 21 national networks, is a pan-European initiative dedicated to fostering collaboration between mathematics researchers and the industrial sector. This presentation introduces EU-MATHS-IN, its mission, and its role in advancing industrial mathematics across Europe by:

• Creating strategic connections among national networks and research centers.

• Fostering international cooperation to enhance competitive advantage.

• Promoting public awareness of mathematics' technological contributions.

• Stimulating European partnerships between mathematical research and industry.

Central to EU-MATHS-IN's efforts is the OpenDesk, a one-stop-shop designed to streamline and amplify the collaboration between mathematical researchers and businesses. The presentation will trace the evolution of the OpenDesk, highlighting its workflow, impact, and benefits. Companies, startups, and researchers alike benefit from this platform: businesses gain access to cutting-edge mathematical expertise to address real-world problems, while researchers enjoy opportunities to engage with practical applications and industry-driven challenges.

The OpenDesk serves as a cornerstone in strengthening Europe's position as a leader in innovation, supporting its industries with tailored mathematical insights and solutions. This session invites participants to explore how the OpenDesk exemplifies the synergy between academia and industry, driving technological progress and fostering economic growth across the continent.

Integrating sequential optimization problems in a multi-objective context

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In several disciplines it is common to plan sequentially, that is several stages are considered in a fixed sequence, carrying decisions from a previous problem into the next one. A typical example is public transport planning in which this sequential approach is followed in practice: Usually, stops are located first, then lines are determined and after that a schedule is fixed. Also in theory, the sequential approach is widely used. Each stage has been considered as an individual optimization problem using the previously computed solution as input of the problem of the next stage.

The objective value of a stage can heavily depend on the input for this stage, that is, a minimizer chosen from the previous stage. The output of a sequential process should thus be evaluated against other possible outputs and even other feasible solutions. This gives rise to a framework where the outcomes of a sequential process are compared with solutions to the so-called *integrated problem* which solves the stages not sequentially, but simultaneously.

So far, the sequential approach has been studied and evaluated problem dependent or only with single objectives. However, the different stages are usually equipped with different, potentially conflicting objectives. Thus, we introduce a multi-objective approach to sequential processes. We consider a general multi-objective sequential process and compare its output to the respective multi-objective integrated problem equipped with the objectives from all stages. We prove weak efficiency of all solutions attained from a sequential process, present assumptions under which (strict) efficiency is achieved and study lexicographic optimality. Furthermore, we derive a cutting plane algorithm from a sequential process. We illustrate our framework for the sequential planning approach in public transport.

Ordered-Median Location Problems in Intermodal Networks

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Modern transportation networks have to accommodate the needs of increasingly diverse groups of users. While some have access to cars, others travel by bicycle, use the public transport infrastructure or walk. Therefore, modern transportation networks are becoming increasingly multimodal, meaning they are usable by a number of potentially very different modes of transport and they allow for the transfer between these modes of transport. We propose a framework to consider this multimodality in a 1-facility location planning scenario.

We model multimodal networks by assigning a length related to each available mode of transport to every edge. Demands in multimodal networks are also assigned a corresponding mobility profile dictating which modes of transport can be used and the order in which they can be used to satisfy the demand.

When a new facility is to be located, it is placed it in such a way that some demand is satisfied as well as possible. What this means exactly differs depending on the facility:
In the case of a medical facility, a center objective is chosen so that even relatively remote locations can quickly get medical attention. This center objective should include every user, independent on their mobility profile.
In contrast, a supermarket might be more interested in being well accessible by a large amount of people, making a median objective more suitable for its placement. Additionally, the reachability of a wholesale supermarket by foot may be considered negligible, while reachability by car may be of higher importance.

To accommodate the different preferences, we consider the well-established ordered-median objective as a unifying framework. Contrary to the non-multimodal case, we construct our objective function using not one but two coupled ordered-median functions. This leads to a parameterizable objective function that also enables us to vary the importance of the different mobility profiles.

Structure-property relationships for nickel-rich cathodes of lithium-ion batteries, using resistor network simulations based on micro-CT image data

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Macroscopic effective properties of battery materials are predominantly influenced by the morphology of their microstructure. In order to bridge the gap between these different length-scales, a stochastic 3D microstructure model is combined with physical simulations on the electrode scale. More precisely, the stochastic model is used to generate virtual, but realistic microstructures of cathodes in lithium ion-batteries. The model is calibrated to tomographic image data and validated with respect to various geometric descriptors and effective transport properties. By varying the parameters of the model, a data base of artificial microstructures with varying densities and particle size distributions is created. Subsequently, the available data is used to investigate structure-property-relationships, which link geometric descriptors of the microstructure to effective properties of the material. In particular, resistor network modeling is used for computing the effective conductivity on the electrode scale, in which the microstructure is represented by a simplified graph structure. This graph structure, the so-called resistor network, is constructed based on virtual and experimental image data on the microscopic scale. Finally, the results are used to validate a previously established empirical formula that uses geometric descriptors of the microstructure to predict the macroscopic effective conductivity.

Topology optimization of two bipolar plate models in hydrogen electrolysis cells

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Hydrogen technologies are essential for achieving climate-neutral mobility and fostering a clean energy sector, with electrolysis cells playing a critical role in hydrogen production. This talk explores the topology optimization of two distinct bipolar plate models in proton exchange membrane (PEM) electrolysis cells.

We first present the two models: the first describes fluid flow within the plate using the Stokes equation with Dirichlet boundary conditions on the fluid surface, while the second introduces a porous medium to relax the original formulation. We state the topological derivative for both models and employ the approach from [1] to numerically compute multiple local minimizers, leading to innovative designs for these plates.

Additionally, we demonstrate that the relaxed model serves as a robust approximation of the Dirichlet model. Through both numerical simulations and theoretical analysis, we show that the relaxed states, adjoints, and a version of the normalized generalized topological derivative converge strongly to their counterparts in the Dirichlet model.

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Theoretical modeling and experimental verification of the electro-thermomechanical coupling of Shape Memory Alloy Hybrid Composites

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Shape memory alloy hybrid composites (SMAHC) are a class of smart composites with the ability to change their shape in response to an external stimulus, making them ideal candidates for material integrated actuators or sensors. Heat or electric current initiates a thermoelastic phase transition in the lattice structure of the shape memory alloy, resulting in a contraction of up to 6 %. Non-axially positioned filaments then lead to a bending deformation of the composite material (compare Figure 1).

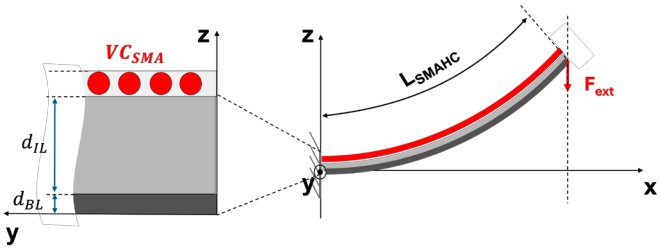

Figure 1: Schematic cross section of a SMAHC with important geometric design parameters

In this work, new results from a multiphysically coupled electro-thermomechanical SMAHC model [1], capable of describing the dynamic shape adaptive behavior on various length scales and also under the influence of external loads and ambient temperatures are presented together with their experimental validation.

Activation and deactivation experiments were performed systematically for different geometries and all material parameters needed for validation purposes were measured. As far as possible, the fully coupled, transient multiphysical model for SMAHC is based on physically motivated, analytical relationships and is fully implemented in python code. For academic purposes it is freely available, its source code and measurement data for its experimental validation for a wide range of mechanical and thermal boundary conditions are published under MIT license.

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Solving Partial Inverse Combinatorial Problems

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Partial inverse combinatorial problems (PICPs) are bilevel optimization problems in which a leader and a follower solve interdependent optimization problems. The follower faces a combinatorial optimization problem, e.g. a shortest path problem or a travelling-salesman problem, while the leader seeks minimal modifications of the weight coefficients in the follower's objective function such that an optimal follower solution includes respectively excludes specified elements. PICPs capture hierarchical decision-making problems like parameter estimation tasks or situations where a planner wants to steer an agent's choice.

In a complete inverse combinatorial problem (CICP), the required and forbidden elements actually specify a unique follower solution. If the follower problem is solvable in polynomial time, the corresponding CICP is again solvable in polynomial time. In contrast, PICPs can become NP-hard despite having polynomial-time follower problems, for example, the partial inverse minimum-cut problem is NP-hard. Considering NP-hard follower problems, the complete inverse mixed integer problem is coNP-complete while determining feasibility for PICPs corresponding to e.g. Hamiltonian cycle or vertex cover is Σ_2^p-complete.

A PICP can be reformulated as a single-level problem with bilinear cuts for feasible follower solutions. For solving a PICP based on this decomposition approach, it suffices to only include cuts for those follower solutions that would otherwise outperform a leader-compliant solution. Thus, we can use a cutting plane method where the separation problem is exactly the follower problem.

We strengthen this single-level formulation by adding linear cuts based on local exchanges. Focusing here on the TSP problem on the lower level, we derive two types of linear cuts: For a path of required edges, this path has to be minimal among all Hamiltonian paths on these vertices. The separation problem for cuts based on such paths is a TSP problem on a smaller instance. A second type of cuts arises from relocating a vertex incident to two required vertices between two other vertices that are adjacent to another required edge. These cuts can be separated by solving an integer program. Our first computational results show the strength of these linear cuts.

Straightforward Computation of Interface-Jacobian and Coupling Sensitivities for Co-Simulation and Solver-Coupling Techniques

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Co-simulation techniques provide a framework for coupling multiple subsystem solvers by exchanging coupling variables at discrete macro-time points. This modular approach allows subsystems to be integrated independently between the communication-time points. Stiff systems or systems with algebraic constraints often require implicit solver coupling schemes to ensure stability and convergence. Implicit predictor/corrector co-simulation approaches need interface-Jacobians (coupling gradients), which describe the sensitivity of subsystem states to variations in coupling variables [1, 2].

Usually, coupling gradients are obtained using a finite difference approximation, requiring additional perturbed subsystem integrations in each macro-step. While conceptually straightforward, finite difference methods increase the computational effort and demand a careful selection of perturbation increments to avoid ill-conditioning and numerical inaccuracies. These issues become especially problematic for large-scale systems with many coupling variables, where the number of perturbed simulations grows rapidly [3].

To address these challenges, analytical low-order approximation formulas for computing interface-Jacobians without requiring any extra subsystem integrations are proposed here. For unconstrained mechanical systems with diagonal mass matrices, closed-form expressions can be derived. For more general systems with arbitrary mass matrices and algebraic constraints, the interface-Jacobian can be obtained by solving a linear system of equations.

This proposed approach offers several advantages. By avoiding additional perturbed simulations, computational costs are reduced significantly, enabling efficient application to problems with a large number of coupling variables. Furthermore, the suggested method is robust against numerical instabilities commonly encountered in connection with finite difference approaches, and it significantly simplifies implementation by removing the need for parallelized integrations. The proposed approximation formulas converge to the exact gradients as the macro-step size approaches zero. Detailed numerical studies are presented, which demonstrate the accuracy and efficiency of the proposed method [2, 3].

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Inverse robust optimization problems and their solution using adaptive discretization methods

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A wide range of robust optimization approaches has been developed to address optimization problems under uncertainty. These methods typically begin with a prescribed uncertainty set and then seek solutions that minimize the impact of uncertainties. However, the construction of an appropriate uncertainty set is crucial: in real-world applications, it is often challenging to determine the set's size and shape a priori. If the uncertainty set is too small, the resulting solution may lack robustness; if it is too large, the cost of robustness can become prohibitive.

In this talk, we adopt a reverse perspective, termed inverse robust optimization. First, we solve the optimization problem for a nominal scenario. Next, we specify a budget that we are willing to allocate to achieve robustness. The objective is then to identify the most robust solution attainable within this budget. In this way, we avoid dependence on an a priori choice of the uncertainty set. We present a general problem formulation and derive results regarding the existence and structure of optimal solutions.

To address the resulting optimization challenges, we demonstrate how these problems can be reformulated as semi-infinite optimization problems. We solve them using adaptive discretization methods. To enhance the performance of these methods, we exploit the bilevel structure of the problems to obtain derivative information. Incorporating this information enables us to design an algorithm with a quadratic rate of convergence.

Normalizing Flow-Enhanced Variational Autoencoder with Neural ODEs for Population Modeling

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Population modeling aims to mathematically represent and predict how individual variability shapes broader population dynamics. In this context, population modeling often deals with time-series data from multiple subjects who share the same model structure, but whose individual parameters are assumed to be samples from a probability distribution. In pharmacometrics, this takes the form of nonlinear mixed-effects (NLME) models, which capture both fixed population-level effects and random individual deviations amid complex nonlinearities and noisy data. The estimation of NLME parameters can be viewed as a form of bilevel optimization, where both population and individual-level objectives are intertwined. A widely used method for this is the Stochastic Approximation Expectation-Maximization (SAEM) algorithm, which iteratively combines stochastic simulation of latent variables with deterministic maximization steps, enabling efficient navigation of complex likelihood surfaces where direct optimization is intractable.

Machine learning, especially neural networks, is increasingly used to improve flexibility and predictive power in population modeling. A common approach integrates them into existing SAEM-based software. However, estimating large networks with SAEM is challenging due to repeated Markov chain Monte Carlo (MCMC) sampling and high computational and memory demands, making it inefficient or impractical at scale. Alternative strategies are therefore needed to incorporate neural architectures into population models.

To address this challenge, we propose a variational autoencoder (VAE) framework with normalizing flows for modeling population data. This approach decouples the estimation process from the SAEM algorithm by leveraging amortized inference, which replaces per-subject sampling with a learned encoder network. In our architecture, the encoder is a transformer model that captures individual variability by processing longitudinal data and mapping it into a structured latent space. The decoder is a neural ordinary differential equation (NODE) that models the temporal dynamics of the system, conditioned on the learned latent variables. The normalizing flow component enhances the expressiveness of the posterior approximation, allowing us to better capture complex latent structures and inter-individual variability.

On simulated data, our model demonstrates predictive accuracy comparable to that of a standard autoencoder. However, by learning a structured, probabilistic latent space, our approach additionally captures individual variability and population-level structure in a principled way. This allows the model to generalize effectively to unseen data and provides richer insight into inter-individual differences, even in the presence of noise and temporal complexity.

Accelerated Permeability Prediction in Fibrous Microstructures Using Deep Learning and CFD Coupling

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The virtual prediction of permeability in fibrous microstructures has become a crucial aspect of multiscale modeling in Liquid Composite Molding Simulation. Conventionally, numerical methods such as the Finite Volume Method (FVM) or the Finite Element Method (FEM) are employed to solve the Stokes equations for creeping flow within Statistical Volume Elements (SVEs). The resulting velocity fields are then volume-averaged, and Darcy's law is applied to compute the effective permeability. While these methods are highly accurate, they are computationally expensive. In response, researchers have recently begun to explore the potential of data-driven machine learning approaches to accelerate such simulations. Although these models offer near real-time predictions, achieving a high level of accuracy—particularly for data that lies outside the training distribution—remains a significant challenge.

This work investigates the use of deep learning—specifically 3D Convolutional Neural Networks (3D-CNNs)—to predict 3D velocity fields from synthetically generated fibrous microscale geometries. A comprehensive dataset of 5607 voxelized microstructures, each containing 400–500 randomly distributed, non-overlapping fibers with varying diameters, orientations, and fiber volume fractions, was generated. Flow fields corresponding to these geometries were computed at varying SVE resolutions: 320^3 voxels (0.5 μm), 160^3 voxels (1.0 μm), and 80^3 voxels (2.0 μm). While 320^3 serves as the reference resolution, the downscaled datasets can serve as a test bed for fast experimentation.

To predict the velocity fields directly from the binary fiber geometries, a 3D U-Net architecture was trained on the reference and downscaled resolutions and benchmarked against MS-Net, a specialized CNN for porous flow.

A key feature of this work is the integration of predicted velocity fields from neural networks as initial conditions in CFD solvers. By using neural network predictions as a running start for OpenFOAM simulations, convergence to the final solution is accelerated—particularly for unseen, out-of-training-distribution geometries. The influence of prediction quality, especially in terms of spatial resolution (80^3, 160^3, or 320^3), on the convergence behavior is currently systematically investigated. Early results showed a promising acceleration in convergence of 14% using low-resolution prediction for unseen data. This hybrid deep learning–CFD approach thus maintains the physical rigor of traditional solvers while reducing simulation time, offering a flexible trade-off between training/inference cost and convergence efficiency.

Multiscale approach to super-resolve X-CT data of crushed fayalite slag, using generative adversarial networks

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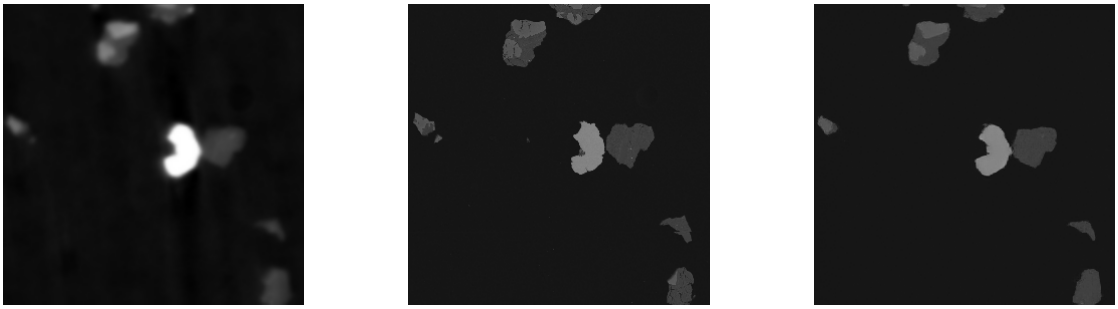
Fayalite slag, a by-product of copper smelting, often retains significant amounts of valuable metals. Because these metals are finely dispersed among complex micro-scale phases, they are hard to extract. Precise micro-structural characterization is therefore critical for designing efficient recycling processes that can minimize losses. X-ray computed tomography (X-CT) provides non-destructive 3D insights but is limited in resolution, whereas scanning electron microscopy-backscattered electron (SEM-BSE) imaging offers high-resolution details for 2D slices.

This study utilizes a multiscale approach to super-resolve 3D X-CT[1] image data of crushed fayalite slag using an enhanced super-resolution generative adversarial network with dual perceptual loss (ESRGAN-DP), as introduced by Song et al., 2023[2]. By training on high-resolution 2D SEM-BSE images, registered to the lower-resolution X-CT data, the network learns to map low- to high-resolution representations, capturing intricate mineral textures and particle boundaries. To obtain super-resolved 3D X-CT data, the trained network is applied slicewise to the X-CT data, generating a super-resolved volume. However, due to the lack of 3D context during the generation of this initial volume, discontinuities occur along the axis orthogonal to the slicing direction. To address this, we combine super-resolved volumes resulting from different slicing directions to produce consistent super-resolved X-CT data (Kirstein et al., 2025)[3].

This multiscale approach improves micro-structural details and segmentation accuracy compared to bicubic-interpolated X-CT, when evaluated against the SEM-BSE ground truth. As shown in Figure 1, the super-resolved X-CT data exhibits improved resolution and transfers the compositional contrast and fine textural details from the SEM-BSE images to the 3D X-CT data. The method effectively bridges scales from 2D high-resolution SEM-BSE slices to 3D X-CT data, combining the strengths of both imaging techniques to enhance multiscale materials characterization for optimization of recycling processes.



(a) (b) (c)

Figure 1: Comparison of measured image data (a,b) and super-resolution result (c): (a) 2D slice of X-CT data (after bicubic upscaling), (b) High-resolution SEM-BSE slice (ground truth), (c) 2D slice of super-resolved X-CT data (using the ESRGAN-DP approach).

[1]The X-CT scans were performed using a TESCAN CoreTOM scanner at the Centre for X-ray Tomography (UGCT) of Ghent University and funded by the European Union's Horizon 2020 research and innovation programme (EXCITE Network) under grant agreement No 101005611.

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Solving adjustable robust problems by bilevel optimization techniques

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In many real-world applications, problems are affected by uncertainty. Robust optimization is one approach to handle such uncertainties but worst-case robustness may yield results that are too conservative. Adjustable robustness allows more flexibility than the classical approach. It distinguishes *here-and-now* decisions that need to be made before the uncertainty is revealed (e.g., investment decisions), and *wait-and-see* decisions that are made later, once the uncertainty is known (e.g., operational decisions). Since many applications allow reactions to revealed uncertainty in some kind of form, this is a very promising approach.

We consider (multicriteria) adjustable robust optimization problems and propose approaches to solve the resulting bi- or trilevel optimization problems. Using (affine linear) decision rules reduces the stages of the optimization problem, but restricts the solution space. Furthermore, we propose a replication ansatz where we solve the adjustable problem for a discretized uncertainty set and compare it with the solution using decision rules. Finally, we demonstrate the use of both approaches in real-world applications.

Computation of Safe Routes to School

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The inclusion of safety aspects in route planning raises new demands on optimization. For example, the safety assessments of paths and crossing points are often ordinal values (like "safe", "relatively safe", "intermediate", "unsafe"). In addition, safety along the route should not be considered additively, as this would correspond to the optimization of average safety along the route. Thus, we obtain an multi-objective optimization problem with ordinal objective functions (safety objectives) and reel valued objectives (e.g. path length). It is known that ordinal optimization problems can be represented by a vector optimization problem, which can be (linearly) transformed into a standard multi-objective optimization problem.

In the EFRE-funded project SAFER (*Sicheres, Algorithmen-basiertes Fußwegerouting*) we are working in collaboration with the company *bueffee* to determine safe, comfortable and short routes for kids to their school. The company bueffee has extensive experience from projects on school route safety and school mobility management. A current focus of the company's research is the behaviour of children at different types of crossings and the development of an innovative safety assessment procedure for traffic planners.

Based on this safety assessment we use ordinal optimization to compute non-dominated paths to school. Depending on the personal security awareness, parents (and kids) will be able to interactively chose and optimize their personal path. We hope to convince more parents to send their children to school by foot and thus reduce the number of parent-taxis. However, using this ordinal path optimization, we will also be able to identify the main routes to each school and possible dangerous crossing points along these routes. These critical crossing points can then be reported to the municipal traffic planners so that they can initiate appropriate construction measures to mitigate them.

Adaptive coupled multiphysics simulations with Trixi.jl

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Coupled multiphysics simulations play a key role in many scientific domains, including fluid dynamics, astrophysics, aeroacoustics, and climate or weather modeling. They are often required to model complex systems involving multiple interacting physical processes. In other cases, they serve to improve computational efficiency by using different models or methods in different parts of the domain. For large-scale applications, efficient coupling algorithms and high-performance implementations are therefore essential.

In this talk, we present recent developments in adaptive coupled multiphysics simulations using the Julia-based numerical simulation framework Trixi.jl. We highlight three representative use cases: embedding Trixi.jl as a submodule into the Fortran-based Earth system modeling framework MESSy, coupling Trixi.jl with the C++-based finite element library deal.II, and performing coupled simulations within Trixi.jl using adaptive model selection. Each of these use cases presents unique challenges, particularly when dealing with cross-language coupling, adaptivity, or heterogeneous hardware systems. We will discuss technical issues encountered, solutions developed, and open questions that remain.

Hybrid Classical–Quantum Pipeline for Crack Detection Using VQLS-Enhanced QSVMs

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This work presents a hybrid classical–quantum pipeline for binary crack detection (crack vs. no-crack), aimed at enhancing automated surface inspection in industrial settings. We combine deep feature extraction with a Variational Quantum Linear Solver (VQLS)-enhanced Quantum Support Vector Machine (QSVM) [1]. A modified ResNet18, pretrained on ImageNet, extracts compact representations from the HairWidthCracks dataset [2], replacing its final layer with a bottleneck output of 31 or 127 features. These features are amplitude-encoded into quantum states and classified using a VQLS-enhanced QSVM, which formulates the SVM dual problem as a linear system solved via variational optimization with a hardware-efficient ansatz. Experiments conducted with the `Qiskit Aer` simulator (10,000 shots per circuit) show that the 127-dimensional features achieve good accuracy while maintaining compatibility with NISQ devices. Our results suggest a promising path toward integrating quantum-enhanced models into real-world industrial inspection pipelines.

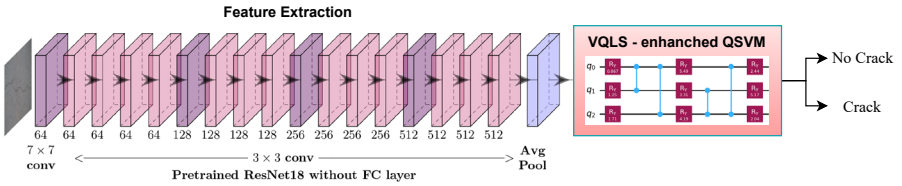

Figure 1: ResNet18 feature extractor with VQLS-enhanced QSVM classifier.

Table 1: Model evaluation metrics for n features = 127.

Metric	**Classical**			**VQLS-enhanced QSVM**		
	Train	Val	Test	Train	Val	Test
Accuracy	0.9300	0.8733	0.8400	0.7925	0.7760	0.7800
Loss	0.1923	0.2838	0.3576	0.2380	0.3257	0.4509

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Predicting the 3D nanostructure of SOFC anodes from 2D SEM images using spatial stochastic modeling and CNNs

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Abstract

The 3D morphology of solid oxide fuel cell (SOFC) anodes significantly influences their macroscopical properties, such as electrochemical performance. Thus, a deeper understanding of the complex 3D geometry of these electrodes is crucial for further optimizing the electrochemical performance of SOFCs. However, the relevant transport processes take place on the nanometer scale, which requires expensive imaging techniques such as 3D focused ion beam scanning electron microscopy (FIB SEM) [1]. To reduce the need for 3D imaging, we present an approach to predict the 3D nanostructure of SOFC anodes based on 2D SEM images via convolutional neural networks (CNNs)[2]. The proposed method utilizes a parametric stochastic 3D model based on tools from stochastic geometry, namely excursion sets of random fields, to generate a large number of virtual but realistic 3D nanostructures. It also employs a physics-based SEM simulation tool [3] to obtain the corresponding 2D SEM images. In combination with the underlying model parameters, a large dataset can be generated to train CNNs. By doing so, we can reconstruct the 3D nanostructure from 2D SEM images by drawing realizations from the stochastic geometry model with the predicted model parameters. In addition, we conducted an error analysis on key geometrical descriptors to quantitatively evaluate the accuracy and reliability of this stereological prediction tool.

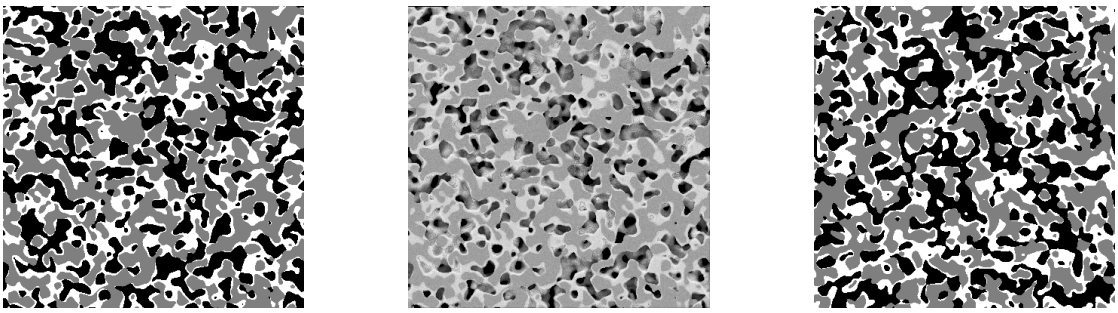

Figure 1: Top slice of a realization drawn from the stochastic 3D model with sampled ground truth parameter vector (left), its corresponding simulated SEM image (middle), and a slice of a realization drawn from the stochastic 3D model with parameter vector predicted by the CNN (right).

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A Mixed-Integer Linear Programming Approach for On-Demand Electric Shuttle Routing with Time Windows and Charging Constraints

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The increasing need for adaptable and sustainable urban transportation solutions has piqued interest in on-demand mobility services. Electric vehicles (EVs) are promising candidates for eco-friendly transit services; however, their operational characteristics, including limited range and recharging requirements, pose considerable challenges for real-world applications. This paper discusses the operational planning and scheduling problem for an on-demand passenger shuttle service using a fleet of heterogeneous electric vehicles (agents). Herein, fleet agents operate within a road network of depots, concurrently acting as charging stations, and pickup/delivery locations. The primary objective is to ensure that all customer requests are fulfilled, each characterized by a specific pickup and delivery location, a number of passengers, and a designated service time window, while minimizing the cumulative travel time of the fleet.

This problem represents an advanced variant of Vehicle Routing Problems (VRPs) that combines elements of the Pickup and Delivery Problem with Time Windows (PDPTW) and the Electric Vehicle Routing Problem (EVRP). Herein, we propose two Mixed-Integer Linear Programming (MILP) formulations to model this EVRP-PDPTW problem, considering agent availability, pickup and delivery requests with time windows, vehicle capacity limits, and battery State of Charge (SOC) constraints. We provide detailed descriptions of both formulations, then implement and compare them to determine their viability in realistic scenarios. Furthermore, we introduce a prototype web-based service to streamline the process of managing customer requests, which is a prerequisite for implementing the on-demand shuttle service on the campus of the University of the Bundeswehr Munich. Small-scale experiments are conducted to validate the operational efficacy of the models and offer insights into potential enhancements for large-scale applications. Finally, we present the limitations of current approaches and discuss suggestions for future research.

A hypervolume-based method for multi-objective two-stage robust optimization problems

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We consider two-stage robust mixed integer programming problems with finite uncertainty sets, where a subset of the decision variables – referred to as the first-stage variables – is shared across all scenarios. Assuming a minimization problem, the goal is to determine the values of these first stage variables such that the worst-case objective value among all scenarios is minimized. In the single-objective case, the resulting min-max-min problem can be reformulated to a single-stage minimization MIP by introducing an auxiliary real variable and then solved with well-known column-and-constraint generation methods. In the multi-objective setting, however, optimizing the worst-case nondominated set introduces additional complexity. Depending on the choice of the quality indicator for evaluating the nondominated set, an equivalent reformulation into a single-stage MIP is often not possible anymore. In our work, we approximate the hypervolume indicator – the most-studied quality indicator in the multi-objective optimization literature – using a grid-based subdivision of the objective space, which allows a reformulation as a single-stage MIP. We detail this formulation and present acceleration techniques to improve computational efficiency. We test our method on two-stage robust multiobjective versions of the selection problem, the assignment problem, and the knapsack problem.

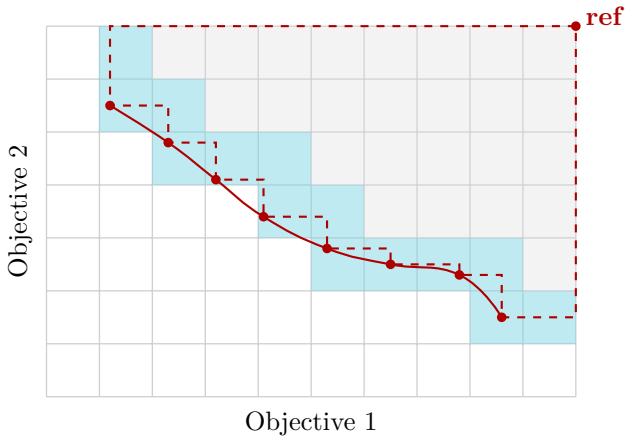

Figure 1: Grid-based subdivision of the objective space for one scenario. Nondominated points are shown in red, and the dashed red line indicates the border of the dominated hypervolume. Activated grid cells are shown in gray, while blue cells are not activated, but contribute to the dominated hypervolume.

The OSCAR computer algebra system

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OSCAR is an innovative **O**pen **S**ource **C**omputer **A**lgebra **R**esearch system that powers cutting-edge computations in algebra, geometry, and number theory. Written in Julia, OSCAR integrates powerful tools from diverse mathematical areas to address even the most complex computations.

Coupling tools from different fields – and implemented in various languages, including C, C++, Perl, and also domain specific ones like GAP and Singular – is a core aspect of our work. We will explain how using Julia helps us to do this efficiently and effectively, both in terms of development resources and execution performance.

Data exchange and serialization are central to our system and are required at multiple levels: of course for communication between components inside a single process as in the previous paragraph; but also for use in parallelized computations across processes on a single machine; for distributed computations across multiple machines; and also for the persistent storage of computational results (e.g., databases of algebraic objects arising from research). We will discuss some of the challenges we encountered – both general and specific to our use case – and how we are addressing them.

Computational Dynamics towards Artificial Intelligence

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The integration of artificial intelligence (AI) – especially large language models (LLMs) – into engineering disciplines is changing the way complex engineering problems are solved, particularly in the field of multibody dynamics (MBD). Despite their potential, engineering tasks are underrepresented in current LLM datasets and research, as they require a deep understanding of mathematics, a combination of textual, visual, and numerical data, and the use of approximations rather than exact solutions. Addressing these challenges, this work introduces a novel framework for automating the generation and validation of simulation models in mechanical engineering, with a focus on MBD problems.

The proposed framework is based on parametrized models with ground truth solutions to create extensive test cases, enabling systematic evaluation of LLM-generated Python-based simulation models within our simulation framework Exudyn. A specialized approach combining in-context learning and specialized retrieval-augmented generation (RAG) significantly enhances performance in simulation model generation. Within systematic tests with 350 simulation models, we could demonstrate the potential of this framework to automate the assessment of LLMs regarding engineering tasks and how to enable natural language interaction with simulation tools. In particular, we could show that best performing LLMs such as QwenCoder (32B) are able to generate 91.7% correct simulation models and 99.4% models without syntax errors. However, more complex tasks, such as flexible bodies, simulator coupling, and advanced user functions, remain challenging for current LLMs and are identified as future research directions.

Within an advanced approach, LLM agents are built to generate MBD models and to perform self-validation through predefined evaluation methods, suitable to distinguish correct from intentionally wrong models. Evaluation results using the F1-score reveal that most tested LLMs can distinguish between correct and incorrect models on a statistics basis, while the best-performing models achieve a score above 0.7, representing a substantial gap between true and false positives.

This work will also shortly highlight the role of deep learning in MBD through methods like SLIDE, which predicts dynamic responses in MBD systems with speedups of up to a million times compared to conventional simulations, incorporating an error estimator for detection of out-of-training application of the method. By integrating AI into simulation and modeling, this research highlights the disruptive potential of AI in engineering and paves the way for future applications in the optimization and solution of open technical problems.

Reduced Order Models in Wheel-Rail Applications

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This work presents a physics-based wear prognosis framework for wheel-rail contact systems, grounded in a Reduced Order Model (ROM) derived from high-fidelity Finite Element Method (FEM) simulations. The ROM captures the essential nonlinearities of 3D frictional contact mechanics, including normal contact pressure distribution and tangential slip under dynamic loading. Prognosis is achieved by coupling this FEM-based ROM with SIMPACK, a multi-body simulation software, which enables efficient and precise evaluation of contact pressure distribution between the wheel and the rail. This in turn is highly important for an accurate prediction of wear evolution, while maintaining computational efficiency suitable for real-life applications. This methodology supports predictive maintenance strategies in railway systems, offering a robust and interpretable tool for assessing drivetrain health and optimizing service intervals.

Multiscale Coupling for the Usage-Specific Simulation of Battery-Electric Vehicles

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The transition towards electrified mobility demands addressing new technological challenges, with the traction battery emerging as a critical component that determines the reliability and operational efficiency of vehicles. Therefore, understanding the performance of the battery under real-world operating conditions is crucial for driving the continuous improvement of current and future battery system designs and, thus, for increasing the consumer acceptance. To address this issue, this work introduces a novel framework that couples a region- and usage-dependent vehicle simulation with battery models incorporating both high fidelity electrochemical approaches and effective surrogate models. The objective is to identify the optimal model complexity for approximating the battery state in real time during operation.

Various models for battery cell simulation were considered in this work, ranging from the detailed electrochemical simulation tool BEST to surrogate models of varying complexity, including both AI-based methods and physics-based approaches. Among these, the physics-based equivalent circuit model was found to be well-suited for efficiently estimating the battery cell state based on its electrical characteristics. Using the dual polarization setup, which consists of the open-circuit voltage, one resistance element and two RC pairs connected in series, polarization effects on two distinct time scales were captured, accounting for both slow diffusion-related dynamics and fast ohmic-loss effects. Alongside the modeling approach, parameterization strategies were introduced, making use of diagnostic test data to calibrate the model parameters. As part of a full-vehicle simulation, the battery pack power was estimated by scaling the simulated single-cell power by the total number of cells, assuming identical cell behavior and uniform current distribution within the pack. Ultimately, the battery pack simulation was coupled with the already established software tool VMC Simulation, allowing the battery state to be monitored during realistic driving operations.

Dual-Mode Model Predictive Motion Cueing for Robot-Based Driving Simulators

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The utilization of interactive driving simulators has witnessed a surge in popularity, emerging as a valuable and highly efficient instrument across a myriad of applications, including driver training, vehicle dynamics design and development. However, the interpretability and validity of such studies are considerably influenced by the precise replication of the simulated vehicle movements and the extent of driver immersion. It is therefore evident that motion cueing algorithms represent a crucial element within the context of interactive driving simulation systems, as they facilitate the generation of realistic motion feedback based on driver interaction with the simulated environment. These methodologies for controlling motion platforms are employed to emulate the acting accelerations and angular velocities within the constraints of the driving simulator. This process replicates the physical dynamics of a vehicle in motion. In recent years, there has been a proliferation of model predictive control (MPC)-based algorithms that have emerged as an alternative to the well-known classical washout algorithms [1],[2]. MPC facilitates explicit consideration of the workspace and offers more intuitive parameterization. Nevertheless, ensuring stability within this optimization-based control framework remains a challenging task. The present paper expounds upon a dual-mode MPC concept, which has been developed for the purpose of ensuring stability for interactive driving simulators. The employment of an invariant set for state feedback as a constraint in the optimization problem has been demonstrated to effectively address workspace and actuator limitations. The efficacy of the proposed approach is demonstrated via a case study employing the interactive robot-based driving simulator RODOS®, which showcases the feasibility of this method for a broad range of human-in-the-loop simulation studies.

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On Subproblem Tradeoffs in Multiobjective Optimization

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Multiobjective programs (MOPs) model decision problems governed by multiple and conflicting objectives that arise in many areas of human activity such as resource management and engineering design. In the presence of conflict, a unique optimal decision is not available. Rather, the decision maker (DM) is presented with a set of non-improvable decisions known as efficient solutions and with the outcomes of these decisions known as Pareto points. The final goal for the DM is to apply preferences, that are not contained in the MOP model, and select a preferred efficient solution as the final decision to be implemented. Solving MOPs therefore involves an optimization stage to compute the efficient and/or the Pareto set, and a decision stage to conduct a search for a preferred efficient solution and/or Pareto outcome.

The difficulty in performing the optimization stage results from the size of the MOP and the type of variables, constraint and objective functions in the mathematical model. In the decision stage, the search for a preferred efficient solution is likely to be manageable for bi- or triobjective programs but becomes challenging for MOPs with more objectives regardless of their type. To resolve these challenges, one of the main research directions has been to decompose the original MOP into subproblems (sub-MOPs), each with a smaller number of criteria. The sub-MOPs are then coordinated to guarantee that by only computing their efficient sets, the efficient set of the MOP can be retrieved. Decomposition and coordination (D&C) methods for MOPs often rely on classical tradeoffs that are defined between two objective functions. We develop a D&C methodology to support decision making for complex MOPs composed of sub-MOPs, and to allow the DM to quantify tradeoffs between the sub-MOPs rather than only between their specific objectives. To accomplish this, we use our results on bivariate achievement scalarizing functions (BASFs), which make the reference point in achievement scalarizing functions a variable. BASFs allow us to define *subproblem tradeoffs*, which measure tradeoffs between entire subproblems as opposed to between individual objective functions. These subsystem tradeoffs are provided by a bilevel MOP solved over the efficient sets of the sub-MOPs. While bilevel MOPs are hard to solve, we believe this difficulty is worthwhile since the proposed bilevel MOP enriches the decision stage with valuable information that other D&C methods cannot provide. However, we formulate an auxiliary MOP which circumvents the difficulties while still conceptually employing the bilevel MOP. We illustrate our new concepts and methods on a case study of disaster relief.

Tools for High Performance Treatment of Coupled Problems

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Fraunhofer SCAI develops innovative methods in computational science and respective software tools. SCAI combines mathematical and computational knowledge with a focus on efficient algorithms to bring benefits to customers and partners in industry.

In this presentation we will focus on high performance computing aspects in the approximation of coupled problems via some of SCAI's software tools. In particular, we will report on the SAMG linear solver library [1], its use within the MESHFREE fluid dynamics simulator [2], the co-simulation framework OCoS [3], and the general simulator platform PUMA [4]. We will demonstrate key performance features of these tools in industrial application settings involving the coupling of multiple compute clusters and GPU acceleration.

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Coupling of fields, scales, dimensions and models in forward and backward analyses for crucial applications in engineering and the applied sciences

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Coupled problems are ubiquitous in all fields of engineering and the applied sciences. In the past, many such problems have nevertheless been treated as single-field problems, as adequate and powerful formulations as well as computational approaches and platforms were lacking to tackle such real-world coupled problems in available time scales. In recent decades, this picture has fortunately changed, and huge progress has been made. Hence, nowadays one only needs to resort to single-field problems when such models are sufficient to answer the relevant questions, and one can aim for including all different coupling effects when needed. Nevertheless, there is still a huge demand for more powerful methods that are both theoretically sound, robust, and efficient, for a huge variety of challenging problems.

In this talk, we will take an application-motivated point of view, i.e., we will start by showing different applications where such coupling effects are crucial for highly relevant questions. A focus here will be on the fascinating field of Biomedicine (where novel physics-based computational approaches have the potential to create a paradigm shift in health care, towards real individualized, patient-specific medicine). From there, we will not only demonstrate the necessity to couple fields, but also the coupling of different scales, dimensions, and models. We will sketch the different approaches that we have developed over the years for such problem scenarios. We will also demonstrate how such couplings can be very beneficial when the quantification of uncertainties is necessary (which is obviously essential in the medical field but also in other domains) or when backward analysis (or inverse analysis/parameter identification) is important.

Polynomial Matrix Inequalities in Structural Optimization

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This talk summarizes our work on using semidefinite programming methods for the optimal design of truss and frame structures.

The first part focuses on an industrial application involving thin-walled composite tubes reinforced by modular truss structures [1]. While these carbon-fiber components offer excellent stiffness-to-weight ratios, wall instabilities limit their use in dynamic environments. We formulate the design task as a large-scale linear semidefinite program that minimizes reinforcement weight while enforcing lower bounds on vibration frequencies and manufacturing stiffness. The entire process—from optimal design accelerated by Schur decomposition, to prototype production using 3D printing, and subsequent verification and validation—will be discussed.

The second part addresses models with bending effects, where stiffness depends polynomially on design variables, resulting in highly non-convex formulations. We propose a nonlinear semidefinite reformulation solved using the Lasserre moment-sum-of-squares hierarchy. Additionally, we introduce a simple procedure for projecting the relaxed solutions onto the feasible set of the original problem, thereby creating a sequence of feasible upper bounds. When combined with lower bounds from the hierarchy, these offer a computable sufficient condition for global ε-optimality. The approach is demonstrated on problems involving static compliance [2], weight [3], and eigenfrequency-constrained optimization [4]. For all these cases, we achieved certified, globally optimal solutions with a limited number of relaxation levels. This work connects practical engineering design with rigorous global optimization, providing new tools and insights for both industrial applications and theoretical research.

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Speakers in Alphabetical Order

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