KLAIM 2021

Kaiserslautern Applied and Industrial Mathematics Days

KLAIM 2021, October 11 to 13, 2021

Book of Abstracts

www.itwm.fraunhofer.de/klaim_en

Table of Contents

Welcome to KLAIM 2021!

October 2021

Dear Participants,

A cordial welcome to all of you – those who have come to Kaiserslautern and those who will participate online! We are really glad that eventually it became possible to organize this conference on-site, with hopefully many opportunities for scientific exchange and lively discussions.

With this new conference format, we want to stake a claim for applied and industrial mathematics by providing a forum for applied mathematicians from academia, research labs and industry to exchange ideas and to showcase recent results. The focus of this first edition of KLAIM will be placed on the role of applied mathematics in the development of digital twins.

The event is organized jointly by the Fraunhofer Institute for Industrial Mathematics ITWM and the Department of Mathematics at the TU Kaiserslautern. Provisions for a hybrid format have been made to stream the presentations for those attendees that will not be present on-site.

The program is structured along the three tracks

- Hybrid System Simulation – Classic Modeling and Control Meet Artificial Intelligence.
  This track is organized in collaboration with the ECMI Special Interest Group Math for the Digital Factory.
- Multiscale Methods and Model Order Reduction
- Integration of Optimization and Data Science

Mathematics in Kaiserslautern

Applied and industrial mathematics has a long and remarkable tradition in Kaiserslautern. The Technomathematics program was introduced in Kaiserslautern by Helmut Neunzert in 1979 and since then has spread throughout Germany, Europe and worldwide. Meanwhile, the Department of Mathematics at the TU Kaiserslautern ranks among the top German mathematics departments. It has a high reputation for its research profile and for its international programs at the master and PhD levels. The Fraunhofer ITWM is one of the leading institutes in industrial mathematics worldwide, and from its beginning there has been a strong cooperation between the TU Kaiserslautern and the Fraunhofer ITWM. Celebrating its 25th anniversary this year, the Fraunhofer ITWM has a record of more than 1000 completed projects in collaboration with industry and currently has 350 members, of which around 60 are PhD students. An extensive international network of partners in Oxford, Cambridge, Harvard, Linz, Eindhoven, Gothenborg, at the Texas A&M, the Lawrence Livermore Lab, the Indian Institute of Science in Bangalore and other places complements its profile and supports the ITWM in keeping up with the latest developments in applied and industrial mathematics.

Dankeschön!

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

Finally, a special and warm "Dankeschön" goes to those people who work behind the scenes to make KLAIM 2021 a success: Stephanie Beck, Gesa Ermel, Steffen Grützner, Tobias Mantel, Sarah Miezal, and Esther Packullat.

Anita Schöbel

Bernd Simeon

Scientific Committee

- **Prof. Dr. Anita Schöbel,** Fraunhofer ITWM, Kaiserslautern
- **Prof. Dr. Karl-Heinz Küfer,** Fraunhofer ITWM, Kaiserslautern
- **Dr. Klaus Dreßler,** Fraunhofer ITWM, Kaiserslautern
- **Dr. Konrad Steiner,** Fraunhofer ITWM, Kaiserslautern
- **Prof. Dr. Johan Carlson,** Fraunhofer Chalmers Centre, Gothenburg
- **Prof. Dr. Simone Göttlich,** University of Mannheim
- **Prof. Dr. Axel Klar,** Technische Universität Kaiserslautern
- **Prof. Dr. Sven Krumke,** Technische Universität Kaiserslautern
- **Prof. Dr. Bernd Simeon,** Technische Universität Kaiserslautern
- **Prof. Dr. Alexander -,** FAU Erlangen-Nürnberg
- **Prof. Dr. Stefan Volkwein,** University of Konstanz
- **Prof. Dr. Dietmar Hömberg,** Weierstrass Institute for Applied Analysis and Stochastics Berlin

Program
Monday, October 11, 2021

	Auditorium
14:00	Welcome Sven Krumke (TUK), Anita Schöbel (ITWM), Bernd Simeon (TUK)
14:10	**A.07 On the Numerical Simulation of Elastic and Nonsmooth Mechanical Systems** [1] Olivier Brüls, University of Liege, BE
15:00	**OPTIMIZATION AND DATA SCIENCE**
	A.27 Data Analytics and Optimization in Production and Logistics [1] Alexander Martin, FAU Erlangen-Nürnberg, Erlangen DE
	A.01 Cost vs. Risk – a Bicriteria Approach to Robust Supply Chain Optimization [2] Heiner Ackermann, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE Erik Diessel, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE
	A.17 Data-Driven Robust Optimization using Unsupervised Deep Learning [2] Marc Goerigk, University of Siegen, DE
16:30	Coffee break
16:50	**MULTISCALE AND MODEL ORDER REDUCTION**
	A.10 Allying Physics-based Reduced Models and Physics Informed Data-driven Models into the Hybrid Modelling Paradigm [1] Francisco Chinesta, Arts et Metiers Institute of Technology, Paris, FR
	A.32 Large Deformations of Metal Foams: Dynamic CT Results, Simulations and Modeling [2] Sebastian Rief, Math2Market GmbH, Kaiserslautern, DE
	A.31 3D Image based Stochastic Micro-structure Modelling of Foams for Simulating Elasticity [2] Claudia Redenbach, TU Kaiserslautern, Kaiserslautern, DE Sarah Staub, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE

1) Plenary or track plenary, 45 min. | 2) Contributed talk, 22.5 min. (both including discussions)

Program
Tuesday, October 12, 2021

	Auditorium	Seminar room Z03.07/08
9:00	**A.08 Analysis-aware Defeaturing: the Mathematical Theory** [1] Annalisa Buffa, EPF Lausanne, CH	
9:50	**MULTISCALE AND MODEL ORDER REDUCTION**	**HYBRID SYSTEM SIMULATION**
	A.40 An Efficient Real-time Reconstructor for Extremely Large Telescopes [2] Bernadett Stadler, Johannes Kepler University Linz, AT	**A.16 Combining Real Driving and System Simulation in the Automated Vehicle-in-the-loop: A Development Platform for Automated Driving** [1] Matthias Gerdts, Universität der Bundeswehr München, Neubiberg, DE
	A.24 An Efficient Model Order Reduction Scheme for Dynamic Contact in Linear Elasticity [2] Diana Manvelyan, Siemens AG, München, DE	
	A.12 Dimension Reduction, Homogenization and Simulation of Textile [2] Riccardo Falconi, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE	**A.03 Data-Driven and Cooperative Optimal Trac Control** [2] Urs Baumgart, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE
	A.22 Model Order Reduction Techniques for Multiscale Fatigue Simulations of Short Fiber Reinforced Polymers [2] Jonathan Köbler, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE	**A.06 Radio Network Simulation and AI** [2] Keith Briggs, BT Labs/AIMM project, Adastral Park, UK
11:20	Coffee break	
11:40	**A.38 On using Reduced Order Models in Adaptive Data-augmented Training of Machine Learning Models for Reactive Flow** [2] Felix Schindler, University of Münster, DE	**A.36 A General Framework for Machine Learning based Optimization under Uncertainty and Inverse Problems** [1] Claudia Schillings, University of Mannheim, DE
	A.20 On Modeling and Simulation of Multiscale Problems Related to Catalytic Filters [2] Oleg Iliev, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE	
	A.34 State-Time Formulation to Reduce the Temporal Dimension in Design Optimization [2] Ward Rottiers, Department of Mechanical Engineering, KU Leuven, BE	**A.09 Data-Driven System Simulation: New Trends and Methods in Vehicle Engineering** [2] Michael Burger, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE
	A.25 Precontitioning of Multiphysics Problems using Rational Approximations [2] Svetozar Margenov, Institute of Information and Communication Technologies, BAS, Sofia, BG	**A.19 Time Series Analysis based on Graph Fourier Methods** [2] Tobias Hofmann, Chemnitz University of Technology, DE
13:10	Lunch break	
14:30	**A.05 Multistage Stochastic Optimization via Kernels** (online) Dimitris Bertsimas, Massachusetts Institute of Technology, Cambridge, USA	
15:20	**HYBRID SYSTEM SIMULATION**	**OPTIMIZATION AND DATA SCIENCE**
	A.21 Polyconvex Anisotropic Hyperelasticity with Neural Networks [2] Dominik K. Klein, Technical University of Darmstadt, DE	**A.37 A Machine-learning-based Approach for Finding Recovery-robust Timetables** [2] Alexander Schiewe, TU Kaiserslautern, DE
		A.29 Generalization Through Controlled Optimization [2] Rohit Pochampalli, TU Kaiserslautern, DE
16:05	Coffee break	
16:20	**A.02 Modular Modelling, Modular Simulation, Modular Time Integration** [1] Martin Arnold, Martin Luther University Halle-Wittenberg, DE	
	A.39 Online and Offline Calibration of Digital Twins in the Smart Assembly 4.0 Framework [2] (online) Anders Sjöberg, Fraunhofer-Chalmers Centre, Gothenburg, SE	
	A.33 Generating Dynamic Human Motion with Optimal Control [2] Michael Roller, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE	
18:00	**OPTIMIZATION AND DATA SCIENCE**	
	A.11 Analytics for Zero Hunger [1] Dick den Hertog, University of Amsterdam, NL	
19:00	Dinner, Atrium at Fraunhofer ITWM	

1) Plenary or track plenary, 45 min. | 2) Contributed talk, 22.5 min. (both including discussions)

Program
Wednesday, October 13, 2021

	Auditorium	Seminar room Z03.07/08
9:00	**MULTISCALE AND MODEL ORDER REDUCTION**	**OPTIMIZATION AND DATA SCIENCE**
	A.26 On Structure-preserving Model Order and Complexity Reduction [1] Nicole Marheineke, University of Trier, DE	
		A.35 The Binary Knapsack Problem with Qualitative Levels [2] Luca E. Schäfer, TU Kaiserslautern, DE
	A.18 Compressed Gas Network Digital Twins [2] Christian Himpe, Max Planck Institute for Complex Dynamical Systems, Magdeburg, DE	**A.23 Tumor Control vs. Normal Tissue Complication Probabilities, the Multicriteria Model and Optimization of Radiotherapy** Karl-Heinz Küfer, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE
	A.30 Combining CFL-like Conditions and Multirate DAE Framework for Applications in System Simulation Software [2] Bernhard Pöchtrager, Austrian Academy of Sciences, Linz, AT	**A.15 Prediction of Mechanical Properties of Heavy Steel Plates** [2] Daniela Gaith, MathConsult GmbH, Linz, AT
	A.41 A Multi-scale Model Hierarchy for Material Flow on Conveyor Belts [2] Jennifer Weissen, University of Mannheim, DE	**A.14 Data-Analysis and Ensemble-Postprocessing for Decision Support in Agronomic Field Management** [2] Jochen Fiedler, Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, DE
	A.13 A Unit Cell Wave Based Reduced Order Modelling Approach for Fast Vibration Response Predictions of Large-scale Finite Periodic Structures [2] Fei Qu, KU Leuven, BE	**A.04 Offer Preparation for Rail Freight Transport** [2] Tim Bergner, TU Kaiserslautern, DE
11:15	Coffee break	
11:30	**A.28 (Localized) Model Reduction with Adaptive Enrichment for PDE Constrained Optimization** [1] Mario Ohlberger, Mathematics Münster, DE	
12:15	Closing remarks	
12:30	Farewell snack	

1) Plenary or track plenary, 45 min. | 2) Contributed talk, 22.5 min. (both including discussions)

Covid-19
Health and Safety Measures

3G rules apply on the premises of the Fraunhofer Center! (In German 3G stands for vaccinated – tested – recovered/geimpft – getestet – genesen). All visitors must be either fully vaccinated, recovered or tested and must also prove this at the reception. The mask requirement in our buildings remains in place.

Principles

- Mouth and nose protection must be worn on the traffic areas inside the buildings. While seated you can remove your masks during the lectures.
- The minimum distance of 1.5 m must be maintained for activities performed in the buildings or on the FhG property.
- Persons with respiratory symptoms (unless cleared by a physician, e. g., cold) or fever should generally not be on the premises.
- Special attention must be paid to hygiene.
- Access for external attendees is permitted only if they can provide proof of a negative rapid test with certificate or proof of vaccination status or convalescent status (3G regulation).
- If a negative test is presented, it must be certified and not older than 48 hours (for antigen tests) or 72 hours (for PCR tests).

In order to ensure that the number of infections among our employees remains very low and to maintain the Institute's ability to work, the sense of responsibility of our employees and managers for their own health and for the health of their colleagues is of particular importance. We therefore ask everyone to continue to pay particular attention to the regulations and offers that have been made.

Notes

Notes

Notes

Cost vs. Risk — A bicriteria approach to robust supply chain optimization

Heiner Ackermann, Erik Diessel

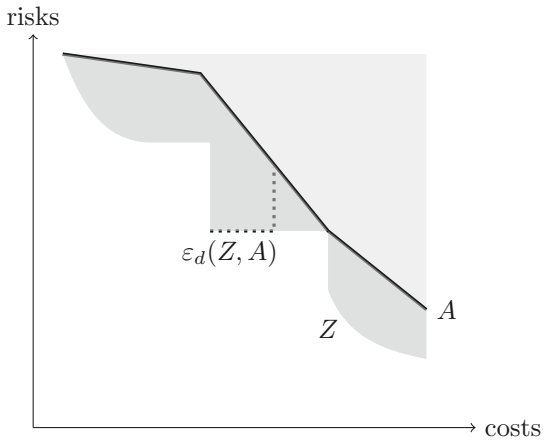
Fraunhofer Intstitute for Industrial Mathematics ITWM,
Fraunhofer-Platz 1, 67663 Kaiserslautern, Germany,
{heiner.ackermann, erik.diessel}@itwm.fraunhofer.de

The continuous and reliable supply of inexpensive raw materials is of great importance for the success of manufacturing companies. However, supply chains face various uncertainties such as political crises, severe weather events, earthquakes, etc., which threaten the availability and flow of material. Therefore, improving the resilience of such networks is essential for manufacturing companies to limit the impact of potential supply disruptions. For sure, increasing the resilience of a supply chain will likely increase purchasing costs due to additional supply points, larger inventories and other proactive countermeasures. Thus, manufacturing companies face a bicriteria optimization problem: Minimize supply costs while simultaneously maximizing resilience.

In this talk, we model the resilience of a supply chain in the framework of adjustable robust optimization and measure it as the amount of shortage in a worst-case failure scenario after the performance of an optimal mitigation. Our approach results in a bicriteria mixed-integer convex program.

For this class of problems, we present a novel algorithm approximating the Pareto frontier. The method has a nice geometric interpretation and applies to arbitrary bicriteria mixed-integer convex programs. The algorithm iteratively generates an approximation consisting of segments by using convex combinations of two solutions sharing an assignment to the discrete variables.

We conclude with a case study of a supply chain operated by a global manufacturer of fast-moving consumer goods.



Modular modelling, modular simulation, modular time integration

Martin Arnold

Martin Luther University Halle-Wittenberg, Institute of Mathematics
martin.arnold@mathematik.uni-halle.de

Network approaches are a quasi-standard for the modelling of complex systems in engineering. They support in a natural way to combine component models of different types including data-driven approaches that are trained by machine learning techniques (*hybrid* system simulation).

Large scale models are typically composed of (nested) substructures, some of them being equipped with specially tailored numerical solvers. The coupling of different subsystem solvers results in modular simulation techniques that fit well to standard process chains in virtual product development but may cause numerical problems in time integration.

We will discuss the stability and convergence of such modular time integration methods using techniques that are known from the analysis of time integration methods for differential-algebraic equations (DAEs). The results of these theoretical investigations will be illustrated by numerical tests for coupled systems in multibody system dynamics.

Data-Driven and Cooperative Optimal Traffic Control

Urs Baumgart[1], Michael Burger[1]

[1]) Fraunhofer Institute for Industrial Mathematics ITWM
{urs.baumgart,michael.burger}@itwm.fraunhofer.de

In view of increasing traffic volumes, accompanied by traffic jams and negative environmental impacts, intelligent mobility solutions are becoming more and more important. At the same time, today's vehicle technology and mobility infrastructure allow to collect and to transmit large and comprehensive data, especially in the light of emerging and maturing communication technologies, such as 5G.
We study approaches to use (real-time) data, communicated between cars and infrastructure, to improve and to optimize traffic flow in the future and, thereby, to support holistic, efficient and sustainable mobility solutions.
To set up virtual traffic environments ranging from artificial scenarios such as the prominent ring road experiment [1] up to complex real world road networks, we use microscopic traffic models. In these models, single cars and their longitudinal dynamics are modelled via coupled systems of ordinary differential equations (ODEs).
We apply different control methods, in order to teach controllers (agents) to guide certain vehicles or to control infrastructural guidance systems, such as traffic lights. The controllers obtain real-time information from other vehicles and, potentially, infrastructure systems and aim to improve the traffic flow for all vehicles in the considered network in a cooperative way. Control methods include model predictive control (MPC) approaches and optimal control algorithms as well as data-driven methods such as Reinforcement Learning (RL) [2]. RL-based approaches can also be applied in a model-free set-up without knowledge of the dynamics. While such data-driven methods have shown to be able to increase the controller's performance in several traffic applications, their solutions may lack of interpretability, and, more important it remains challenging to guarantee stability and robustness. We compare, analyse and discuss the different control approaches in terms of performance, accuracy, robustness and safety, even under extreme and rare traffic conditions, for dedicated road networks and scenarios.

References

[1] Sugiyama, Y., Fukui, M., Kikuchi, M., Hasebe, K., Nakayama, A., Nishinari, K., Tadaki, S.-i., and Yukawa, S. (2008). Traffic jams without bottlenecks—experimental evidence for the physical mechanism of the formation of a jam. *New Journal of Physics*, 10(3):033001.

[2] Baumgart., U. and Burger., M. (2021). A reinforcement learning approach for traffic control. In *Proceedings of the 7th International Conference on Vehicle Technology and Intelligent Transport Systems - VEHITS*, pages 133–141. INSTICC, SciTePress.

Offer Preparation for Rail Freight Transport

Tim Bergner[1], Sven O. Krumke[2]

[1]) TU Kaiserslautern
bergner@mathematik.uni-kl.de
[2]) TU Kaiserslautern

Rail network operators offer customers the opportunity to reserve train paths for freight trains. When serving a customer request it is common to answer it by a single train path. A joint project between DB Netz AG and the optimization group of TU Kaiserslautern is about the problem of computing multiple options from which the customer may choose one. The train paths offered should be both as good and as different as possible. To achieve this we mainly focus on the following properties of the paths: their distance, duration, and deviation of desired departure or arrival times. We also consider the geographic courses as they strongly influence the perceived difference.

When computing the train paths, the existing traffic has to be taken into account. That is, every such path must not conflict with other trains that are already scheduled in the network. Thus, we are essentially given a multicriteria, time-dependent shortest path problem. The requirement of good paths translates to finding efficient solutions which we obtain by weighted sum scalarization. To obtain the desired different paths we first determine sufficiently many efficient ones and select a diverse set of these.

In the talk we concentrate on the computation of shortest paths within this setting. This problem is not just NP-hard in theory but also challenging to solve on real world instances. Different adaptions and improvements of standard shortest path algorithms are necessary to speed up the computation to a point where it becomes practically useful.

Multistage Stochastic Optimization via Kernels

Dimitris Bertsimas[1], Kimberly Villalobos Carballo[2]

[1]) Boeing Professor of Operations Research, Massachusetts Institute of Technology, Cambridge, MA 02139, dbertsim@mit.edu
[2]) Operations Research Center, Massachusetts Institute of Technology, Cambridge, MA 02139, kimvc@mit.edu

We develop a non-parametric, data-driven, tractable approach for solving multistage stochastic optimization problems in which decisions do not affect the uncertainty. The proposed framework represents the decision rules as elements of a reproducing kernel Hilbert space and performs functional stochastic gradient descent to minimize the empirical regularized loss. By incorporating sparsification techniques based on function subspace projections we are able to overcome the computational complexity that standard kernel methods introduce as the data size increases. We prove that the proposed approach is asymptotically optimal for multistage stochastic optimization with side information. Across various computational experiments on stochastic inventory management problems, our method overcomes the curse of dimensionality and remains tractable when the data size is large. Lastly, by computing lower bounds on the optimal loss of the inventory control problem, we show that the proposed method produces decision rules with near-optimal average performance.

Radio network simulation and AI

Keith Briggs[1]

[1]) BT Labs & AIMM project
keith.briggs@bt.com

Simulation techniques have long played a role in the planning and management of radio access networks (RAN), i.e. cellular radio systems. These techniques have now evolved to a level of sophistication that some of them can rightly be called digital twins. These incorporate many aspects of the layout and traffic distributions of a real RAN, eventually one conforming to the new standard defined by the O-RAN Alliance. In the AIMM project (a multi-partner collaboration under the CELTIC-NEXT scheme, http://aimm.celticnext.eu), we are taking this a step further by integrating AI techniques into the simulator in order to predict the performance of the RAN when under AI management and control. In this talk I will describe some of the AIMM activities, with a discuss of software design issues and examples of simulation outputs.

On the Numerical Simulation of Elastic and Nonsmooth Mechanical Systems

Olivier Brüls and Alejandro Cosimo

Department of Aerospace and Mechanical Engineering, University of Liège
Liège, Belgium
[o.bruls,acosimo]@uliege.be

Today, there is a growing interest in the simulation of mechanical systems whose behaviour is strongly affected or even fully driven by structural elastic effects and nonsmooth contact interactions. For example, lightweight robots, such as collaborative robots, exhibit link and joint flexibility and are designed to enter in contact with their environment and with human operators; soft robots are actuated through deformable components, such as inflated membranes or cables, for the purpose of locomotion and/or grasping tasks; and the manipulation of soft components such as cables or textiles is particularly important for the automotive and the composite industry.

Despite great progresses over the last decades, flexible multibody dynamics and nonsmooth contact mechanics mostly evolved as separate branches in computational mechanics. On the one hand, geometric methods (in particular, Lie group methods) played a central role in the development of powerful formalisms for flexible multibody systems as well as for the development of robust space and time discretization algorithms. On the other hand, the theory of nonsmooth contact dynamics offers a rigorous mathematical framework for the treatment of unilateral constraints and friction models in mechanical systems along with robust time-stepping integration procedures. In the aforementioned application areas, however, there is a need to develop a more unified simulation framework conciliating these two approaches.

This talk addresses open questions that arise in the simulation mechanical systems involving both structural elastic effects and nonsmooth contact models. A geometric finite element approach is proposed to formulate the semi-discrete equations of motion with bilateral and unilateral constraints. The role of the constraints at position, velocity and acceleration levels is discussed and a nonsmooth generalized-α time integration scheme is presented. This algorithm leads to a numerical solution which simultaneously satisfies the unilateral and bilateral constraints at position, velocity and acceleration levels. A few numerical examples are exploited to illustrate the properties of the method, such as its ability to capture nonsmooth behaviours, geometric nonlinearities and vibration phenomena in an accurate and stable manner.

Analysis-aware defeaturing: the mathematical theory

Annalisa Buffa[1], Ondine Chanon[1], Rafael Vazquez[1]

[1]) Chair of Numerical Modelling and Simulation, EPF Lausanne
annalisa.buffa@epfl.ch

Defeaturing consists in simplifying geometrical models by removing the geometrical features that are considered not relevant for a given simulation. Feature removal and simplification of computer-aided design models enables faster simulations for engineering analysis problems, and simplifies the meshing problem that is otherwise often unfeasible. The effects of defeaturing on the analysis are then neglected and, as of today, there are basically very few strategies to quantitatively evaluate such an impact. Understanding well the effects of this process is an important step for automatic integration of design and analysis. We formalize the process of defeaturing by understanding its effect on the solution of the Laplace equation defined on the geometrical model of interest containing several features. We derive a simple, efficient and reliable a-posteriori estimator of the error between the solutions of the exact and the defeatured geometries and demonstrate its performance with a few examples.

Data-Driven System Simulation: New Trends and Methods in Vehicle Engineering

Michael Burger[1], Klaus Dreßler[1]

[1]) Fraunhofer ITWM
{michael.burger, klaus.dressler}@itwm.fraunhofer.de

In this contribution, we give an overview on current developments, new trends and challenges in the field of vehicle engineering. We start with a review and summary of classical mathematical methods for computed-aided engineering (CAE) of vehicles, which built a dedicated backbone for many modern techniques. In particular, in the considered automotive field, the availability of data has been increasing strongly for years; this applies not only to quantities measured directly on a vehicle, but also to information and data describing the environment. At the same time, technologies for data acquisition, data management, communication and computational data processing are also continuously improved and further developed. Today, both allow to derive more and more valuable knowledge and information from existing data sets using suitable methods and tools from data-based mathematics. Moreover, the combination of classical system simulation with data analytics and methods and tools from artificial intelligence (AI) reveal the potential to significantly improve different stages in the vehicle development process. We discuss and highlight those new trends and combinations on the basis of selected engineering examples:

- AI methods in vehicle engineering: Identification of usage profiles with vehicle field-monitoring data and derivation of highly efficient surrogate models.
- Derivation of customer- and region-specific durability loads and enery demands for modern vehicles, on the basis of geographic data and simplified simulation models.
- Hybrid environmental and system simulation for (interactive) driving scenarios.

We illustrate these application examples, we discuss the properties of the underlying mathematical models and tools and we address, in particular, the corresponding optimal model complexity for specific tasks and targets. We highlight current (mathematical) challenges and consider future options and potentials.

Allying physics-based reduced models and physics informed data-driven models into the hybrid modelling paradigm

Francisco Chinesta[1], Victor Champaney[1], Elias Cueto[2]

[1] PIMM Lab at Arts et Metiers Institute of Technbology, ESI Group Chair, France
Francisco.Chinesta@ensam.eu
[2] I3A at University of Zaragoza, Spain
ecueto@unizar.es

World is changing very rapidly. Today we do not sell aircraft engines, but hours of flight, we do not sell an electric drill but good quality holes, ... and so on. We are nowadays more concerned by performances than by the products themselves. Thus, the new needs imply focusing on the real system subjected to the real loading that it experienced until the present time in order to predict the future responses and in this manner, anticipate any fortuity event or improve the performances. Here, usual modeling and simulation techniques are limited because of the fact that a model is sometimes no more than a crude representation of the reality. Artificial Intelligence irrupted and became a major protagonist in many areas of technology and society at the beginning of the third millennium, however many times it require impressive training efforts (incredible amount of data, most of them inexistent, difficult to collect and manipulate, extremely expensive in time and resources).

A highway to circumvent these difficulties and successfully accomplishing the most efficient (fast, accurate and frugal) generation of information and knowledge facilitating a real-time decision-making in engineering consists of a hybrid paradigm combining real-time physics ad real-time data-driven modelling.

From the physics-based modeling viewpoint, an appealing route consists of constructing offline parametric solutions within the so-called PGD. Non-intrusive PGD procedures have been proposed, operating from a number of high-fidelity solutions performed offline, for different choices of the model parameters, among them the SSL-PGD, s-PGD, r-PGD, s2-PGD, ANOVA-PGD, m-PGD, ... Once the parametric solution of the problem at hand is available, it can be particularized online for any choice of the model parameters, enabling simulation, optimization, inverse analysis, uncertainty propagation, simulation-based control, ... all them under the stringent real-time constraint.

From the data-driven modeling viewpoint, we will address four main topics: (i) real-time data-assimilation; (ii) physics-aware machine learning technologies able to proceed in real-time and in the low-data limit; (iii) addressing data issues related to the data intrinsic dimensionality, the existence of hidden variables, addressing outliers, noise and missing data, ...; and (iv) the hybridation between the physics-based and the data-driven models for defining efficient dynamics data-driven application systems. Different case-studies will serve to illustrate the potential and prove the performances.

Analytics for Zero Hunger

Dick den Hertog

University of Amsterdam, Amsterdam, The Netherlands

In this talk I will describe a recent optimization project for the UN World Food Programme (WFP). Due to optimization WFP can now feed millions more people. This project was awarded the INFORMS Franz Edelman Award in Spring 2021.

WFP is the largest humanitarian agency fighting hunger worldwide, reaching around 80 million people with food assistance in 75 countries each year. To deal with the operational complexities inherent to its mandate, WFP has been developing tools to assist their decision makers with integrating the supply chain decisions across departments and functional areas. The talk describes a mixed integer linear programming model that simultaneously optimizes the food basket to be delivered, the sourcing plan, the routing plan, and the transfer modality of a long-term recovery operation for each month in a pre-defined time horizon. By connecting traditional supply chain elements to nutritional objectives, we made significant breakthroughs in the operational excellence of WFP's most complex operations, such as Iraq and Yemen. I show how we used optimization to reduce the operational costs in Iraq by 17%, while still supplying 98% of the nutritional targets. Additionally, I show how WPF is using optimization in Yemen to manage the scale-up of the existing operation from three to six million beneficiaries.

When time permits I will briefly sketch how this project fits in the broader *Analytics for a Better World* initiative. Especially the current project in cooperation with the WorldBank to optimize the number and locations of health facilities in Timor-Leste and Vietnam will be briefly explained.

Joint work with: Hein Fleuren (Tilburg University), Koen Peters (WFP, Tilburg University), Sergio Silva (WFP), Tim Sergio Wolter (WFP), Luis Anjos (WFP), Nina van Ettekoven (WFP), Eric Combette (WFP), Anna Melchiori (WFP), Ozlem Ergun (Northeastern University).

Dimension Reduction, Homogenization and Simulation of Textile

G. Griso[1], R. Falconi[2], D. Neusius[2], J. Orlik[2], K. Steiner[2]

[1]) Sorbonne Université, CNRS, Université de Paris, Laboratoire Jacques-Louis Lions (LJLL), F-75005 Paris, France
[2]) Fraunhofer ITWM 67663 Kaiserslautern, Germany
julia.orlik@itwm.fraunhofer.de

In textiles, the behavior of the material is determined by the structural arrangements of the fibers, their thickness and cross-section as well as the properties of the fibers themselves. The friction between yarns also plays a crucial role in the textile behavior. The talk is based on the mathematical modeling, asymptotic dimension reduction and homogenization approaches and is illustrated by examples on different textile structures. This talk summarizes rigorous results of asymptotic analysis and algorithms for simulation of textiles. Some of the theoretical results are validated by experiments.

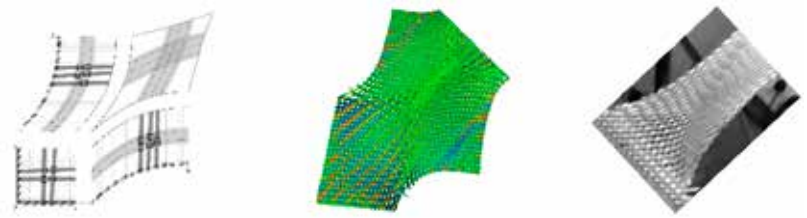


Figure 1: Analysis, Numeric, Experiment

References

[1] Griso, G., Orlik, J., Wackerle, S. Homogenization of textiles. SIAM J. Math. Anal., **52**(2), 1639–1689, (2020)

[2] Griso, G., Orlik, J., Wackerle, S. Asymptotic Behavior for Textiles in von-Kármán regime. J. Math. Pures Appl, **144**, 164–193 (2020)

[3] Falconi, R.; Griso, G.; Orlik, J. Wackerle, S. Homogenization for textile with loose contact. In preparation.

[4] Wackerle, S., Orlik, J., Hauck, M., Lykhachova, O., Steiner, K. The Way to Design a Textile with Required Critical Folding Deformation, Procedia Manufacturing, **Vol. 47**, Elsevier, 174–181 (2020)

A unit cell Wave Based reduced order modelling approach for fast vibration response predictions of large-scale finite periodic structures

Fei Qu[1,2,3], Claus Claeys[1,2], Lucas Van Belle[1,2], Elke Deckers[1,2], Wim Desmet[1,2]

[1] KU Leuven, Department of Mechanical Engineering, Division LMSD, Belgium
[2] DMMS lab, Flanders Make
[3] SIM M3 program, Technologiepark 48, B-9052 Zwijnaarde, Belgium
fei.qu@kuleuven.be

In the past decades, periodic structures and metamaterials in particular have attracted significant attention as innovative noise and vibration control solutions which can combine lightweight requirements with favourable vibro-acoustic performance. To predict their vibro-acoustic performance, periodicity is generally exploited by considering a single finite element unit cell model and calculating dispersion curves. However, to predict the performance in real-life applications, finite structure vibration responses are of interest. Due to the often complex and detailed nature of the unit cells, the unit cell finite element models can be come large, which would rapidly render finite structure models comprised of unit cell assemblies computationally unaffordable. To overcome this problem, in this work, a unit cell modelling approach is proposed to efficiently compute forced vibration responses of finite periodic plates.

To this end, a Wave Based Method rationale is followed [1]. The method belongs to the family of indirect Trefftz methods and it approximates the dynamic field variables using a weighted sum of wave functions, which are free and forced vibration waves of the corresponding infinite plate. By minimising the errors on boundary conditions in a weighted residual sense, a system of equations is obtained and solved for the unknown contribution factors of each wave function. However, unlike the typical Wave Based Method, the analytical wave functions are not available for structures composed of arbitrary unit cell assemblies. Instead, the Wave Finite Element Method incorporating the Generalized Bloch Mode Synthesis is used for efficient calculation of the wave functions by solving a dispersion eigenvalue problem for a single unit cell finite element method. By expanding these unit cell based wave functions through multiplication with the propagation constants, the wave function basis for the finite plate are obtained. The computational efficiency in a comparison with a dynamic sub-structuring approach is investigated for different unit cells.

Acknowledgements

The work has been funded by the project “MOR4MDesign”, which is part of the MacroModelMat (M3) research program coordinated by Siemens (Siemens Digital Industries Software, Belgium) and funded by SIM (Strategic Initiative Materials in Flanders) and VLAIO (Flanders Innovation & Entrepreneurship Agency). The Research Fund KU Leuven is also gratefully acknowledged for its support. The research of L. Van Belle is funded by a grant from the Research Foundation – Flanders (FWO).

References

[1] Deckers, Elke, et al. ”The wave based method: An overview of 15 years of research.” Wave Motion 51.4 (2014): 550-565.

Data-Analysis and Ensemble-Postprocessing for Decision Support in Agronomic Field Management

Jochen Fiedler[1], Michael Burger[1]

[1]) Fraunhofer ITWM
{jochen.fiedler, michael.burger}@itwm.fraunhofer.de

In the agricultural work process, very extensive data can be collected at many points, e.g. spatially resolved yield balances of individual fields. In addition, environmental data and mathematical methods for statistical data analysis and prediction models are constantly being developed. All these factors can be used to support farmers in the diverse and sometimes highly complex decision-making processes of their daily work. In this contribution, we focus on decision support for field management and field cultivation. Depending on soil type, topography, weather forecast, cultivation and yield history, or even regulatory conditions, different courses of action are possible and must often be assessed and re-evaluated by the farmer from day to day. We present mathematical tools and their software implementation that aim at supporting farmers in this process.

As part of the Fraunhofer lighthouse project COGNAC, we are conducting research on the use and statistical analysis of agronomic field data, their aggregation and visual processing, and their combination with environmental information, e.g., topography and weather forecasts. Moreover, we develop methods and procedures to efficiently analyze historical data sets and relate them to field characterizations. This allows a farmer, simply and efficiently, to make comparative analyses of previous strategies, from which, in turn, conclusions for upcoming decisions and tasks can be drawn. Furthermore, we deal with plant growth models for yield prediction, in combination with the so-called ensemble post-processing technique. Those models typically allow to predict yield growth for different crops depending on weather patterns, soil type and numerous other environmental parameters. Due to the complexity of the models, a good calibration is often very challenging in practice. This problem shall be mitigated and partially compensated by the use of ensembles. An ensemble is a collection of predictions which can be obtained from different models or different parameterizations. This approach is a proven state of the art, e.g., for weather forecasts, which has significantly improved the forecast quality in recent years. In our contribution, we demonstrate how such ensembles can be generated for plant growth models and then used to predict yield while quantifying and visualizing the corresponding prediction uncertainty. In addition, different times and amounts of fertilizer application can be comparatively evaluated and analyzed.

Prediction of Mechanical Properties of Heavy Steel Plates

Daniela Gaith[1], Thomas Kaltenbrunner[2], Michael Liebrecht[1,3], Erik Parteder[2]

[1]) MathConsult GmbH
daniela.gaith@mathconsult.co.at
[2]) voestalpine Grobblech Gmbh
[3]) Johann Radon Institute for Computational and Applied Mathematics, Austrian Academy of Sciences

Aiming to deliver a high-quality end product, heavy steel plates, as for example used for structural components in heavy machinery, line pipe and offshore applications, have to meet the desired mechanical properties demanded by the customers. To reach this goal a lot of experience and continuous research and development in each single production step is inevitable. Based on this knowledge, a phenomenological, continuous model predicting mechanical properties like yield and tensile strength of heavy plates within the production range and beyond has been created. In this talk, the underlying concept and the resulting outcome of this predictor are presented.

For reasons of simplification and traceability, the final model describing the production process has been divided into several sub models, each of which describes the influence of a specific production step, i.e. reheating, hot rolling, accelerated cooling and levelling, on the mechanical properties of heavy plates. From the analysis of different data sets, either gained directly from the production or specifically created in a laboratory, in combination with well established metallurgical behaviour, the functional characteristics of the influencing process parameters, such as cooling rate and final cooling temperature, could be identified. A very dominant influence covered in this multidimensional model comes from the chemical composition of the plates. With the help of least squares fitting methods, the appropriate coefficients for these parameter dependent, non-linear models have been elaborated. The resulting predictor provides a detailed understanding of the influence of the process parameters and the chemical composition on the mechanical properties.

The results of the predictor applied to actually produced heavy plates compared to the corresponding measured mechanical properties of these plates show good agreement over the entire range of production. The deviations are attributable to statistical error and sufficiently small, hence the predictor qualifies as reliable pre-production estimator for the mechanical properties of heavy plates.

This predictor offers the opportunity to simulate different production scenarios and consequently optimize the parameter settings leading to the desired mechanical properties. In combination with the accuracy and short computation time, this model could serve as a mature operational tool in the automation process.

Combining real driving and system simulation in the automated Vehicle-in-the-loop: A development platform for automated driving

Matthias Gerdts[1]

[1]) Department of Aerospace Engineering, Universität der Bundeswehr München,
Werner-Heisenberg-Weg 39, 85577 Neubiberg
matthias.gerdts@unibw.de

Automation and autonomy becomes more and more important in many robotics applications, especially for mobile robots, which move automatically in a production site, or for automated cars, which move in the traffic. In this respect we introduce the automated Vehicle-in-the-Loop (VIL), which is a versatile research vehicle combining virtual reality and real automated driving experience at the same time. It provides a testbed for automated and cooperative driving tasks on the basis of an Audi A6. Moreover it is well suited for investigating human-machine interaction, especially in potentially dangerous scenarios.

This talk provides an overview on the technical setup of the VIL and on-going algorithmic control developments such as online path planning using model-predictive control, tracking control, collision avoidance, and control of interacting systems using hierarchies and generalized Nash equilibrium problems.

Deterministic optimal control techniques play a central role in these tasks and to achieve realtime capability and robustness is the challenge. Alternatively, feedback control laws can also be realized through neural networks and reinforcement learning. Attempts in both directions will be dicussed.

Data-Driven Robust Optimization using Unsupervised Deep Learning

Marc Goerigk[1], Jannis Kurtz[1]

[1]) Network and Data Science Management, University of Siegen, Germany
marc.goerigk@uni-siegen.de

Robust optimization has been established as a leading methodology to approach decision problems under uncertainty. To derive a robust optimization model, a central ingredient is to identify a suitable model for uncertainty, which is called the uncertainty set, containing all scenarios against which we wish to protect. An ongoing challenge in the recent literature is to derive uncertainty sets from given historical data.

In this presentation we use an unsupervised deep learning method to construct non-convex uncertainty sets from data, which have a more complex structure than the typically considered sets. We show how the trained neural networks can be integrated into a robust optimization model by formulating the adversarial problem as a convex quadratic mixed-integer program. This allows us to derive robust solutions through an iterative scenario generation process. In computational experiments, we compare this approach to a related approach, which derives uncertainty sets by kernel-based support vector clustering. We find that uncertainty sets derived by the unsupervised deep learning method can give a better description of data, leading to robust solutions that often outperform the comparison method both with respect to objective value and feasibility.

Compressed Gas Network Digital Twins

Christian Himpe[1], Sara Grundel[2], Peter Benner[3]

[1]) himpe@mpi-magdeburg.mpg.de
[2]) grundel@mpi-magdeburg.mpg.de
[3]) benner@mpi-magdeburg.mpg.de
Max Planck Institute for Complex Dynamical Systems Magdeburg
Sandtorstr. 1, 39106 Magdeburg

Modeling, simulation and optimization for digital twins of gas networks is essential to ensure economical energy supply and enable the renewable energy transition. Yet, gas network twins are based on complex compounded mathematical models and potentially large-scale network topologies; thus, for many-query simulations, task-specific compressed twins need to be derived via model order reduction to complete required simulations on-time.

Following a standard dynamic gas pipeline network modeling ansatz, we consider a hyperbolic, nonlinear, parametric partial differential-algebraic equation system as a base model [1]. Since a simulation scenario is fully specified by the transient boundary values, and the relevant simulation results are only certain quantities of interest, the model is specified as an input-output system:

$$E(\theta)\dot{x}(t) = Ax(t) + Bu(t) + F + f(x,\theta), \quad y(t) = Cx(t).$$

For expansive networks, these gas network models become high-dimensional, not least due to their hyperbolicity, and thus prevent a swift repeated simulation. To accelerate simulations, the gas network twins are compressed by model reduction algorithms, that are system-theoretic, to focus on the boundary-value-to-quantity-of-interest mapping, nonlinear, due to the friction and compressor components, and parametric, to regard temperature and gas composition [2].

To recommend model-solver-reductor ensembles for industrial use, we test, benchmark, and compare various reductors for different models and solvers using `morgen` [3], a modular open source simulation platform, which is extensible with custom models, solvers, or reductors, and beyond gas transport to district heating and water networks.

References

[1] P. Benner, S. Grundel, C. Himpe, C. Huck, T. Streubel, and C. Tischendorf. Gas network benchmark models. In *Applications of Differential Algebraic Equations: Examples and Benchmarks*, Differential-Algebraic Equation Forum, pages 171–197. Springer, Cham, 2018. `doi:10.1007/11221_2018_5`.

[2] C. Himpe, S. Grundel, and P. Benner. Model order reduction for gas and energy networks. *Journal of Mathematics in Industry*, 11:13, 2021. `doi:10.1186/s13362-021-00109-4`.

[3] C. Himpe and S. Grundel. `morgen` – Model Order Reduction for Gas and Energy Networks. `https://git.io/morgen`, 2021.

Time Series Analysis based on Graph Fourier Methods

Tobias Hofmann[1], Christoph Helmberg

Chemnitz University of Technology
[1]) tobias.hofmann@math.tu-chemnitz.de

The goal of this talk is to discuss a general mathematical methodology to identify events in high-dimensional time series. In the collaborative research project "Hybrid Societies", we are working in, such time series are generated in practical studies for various applications. For example, we analyze data from autonomous driving experiments where we want to predict the comfort level of the passengers based on numerous physiological and technical parameters. In another collaboration, we investigate motion data in order to optimize robotic behavior and to facilitate natural human-machine interaction.

In all these applications, we aim to learn functional relationships based on high-dimensional input data. For this task, we use discrete graph-based methods for building a finite state transition model. For the analysis, we propose graph Fourier methods which can serve as the basis for kernel regression methods. In contrast to classical regression methods, such approaches may have some advantages when we are interested in specific sequential aspects or when underlying data is linked to some network structure. Bringing these techniques together, we aim to develop new algorithmic methods that answer theoretical as well as practical questions and support human-interpretable time series analysis.

On modeling and simulation of multiscale problems related to catalytic filters

Oleg Iliev[1], Torben Prill[1], Andro Mikelic[2], Robert Greiner[3], Martin Votsmeier[3]

[1]*Fraunhofer Institute for Industrial Mathematics, ITWM, Kaiserslautern*

[2]*University of Lion 1,* [3]*Umicore*

The catalytic membranes can degrade gaseous pollutants to clean gas via a catalytic reaction to achieve green emissions. A catalytic membrane is a three scale porous medium. The walls of catalytic filters are of size of centimeters or millimeters and consist of active (washcoat) particles, inert material and microscale, micron size pores. The washcoat particles are porous material with nanoscale pores. The catalytic reactions are heterogeneous (surface reactions) and they occur within the nanopores. Obviously, simulations at fully resolved pore scale are not feasible. A standard convection diffusion reaction is usually used in the engineering practice with considering (homogeneous reaction within the washcoat. The latter is correct in the diffusion dominated case, when the heterogeneous reaction at nanopore scale can be upscaled to homogeneous effective reaction in the averaged washcoat particles. Upscaling techniques have been considered also from micro to macro scale, but mainly in diffusion dominated regimes. It is known that the same microscale problem can be upscaled to different macroscale equations depending on the characteristic numbers. In this talk we present two studies: (A) Homogenization of reactive flow in the presence of strong absorption in the washcoat particles. Two flow regimes are studied, P_eff = O(1) and P_eff= O(ε^{-1}), and two different upscaled equations are obtained, respectively. The both derived upscaled equations are numerically validated comparing their solution to the solution of the microscale problem. (B) Three-way catalyst material was deposited inside the pores of a ceramic particulate membrane and the pore geometry as well as the distribution of the catalyst in the pores was determined by X-ray -microtomography (CT). On the resulting 3D geometry, the flow field through the pores was computed and the convection diffusion reaction equation in the open pores and the catalyst particles was solved assuming a first order reaction taking place in the catalyst. The conversion computed with the pore scale resolved model was compared to conversion computed with macroscale model used in engineering practice.

Polyconvex anisotropic hyperelasticity with neural networks

Dominik K. Klein[1,*], Mauricio Fernández[2], Robert J. Martin[3], Patrizio Neff[3] and Oliver Weeger[2]

[1]) Cyber-Physical Simulation Group, Department of Mechanical Engineering & Centre for Computational Engineering, Technical University of Darmstadt, Dolivostr. 15, 64293 Darmstadt, Germany
[2]) Access e.V., Intzestr. 5, 52072 Aachen, Germany
[3]) Chair for Nonlinear Analysis and Modeling, Faculty of Mathematics, University of Duisburg-Essen, Thea-Leymann-Str. 9, 45127 Essen, Germany
[*]) Corresponding author, email: klein@cps.tu-darmstadt.de

In the present work [1], two machine learning based constitutive models for finite deformations are proposed. Using input convex neural networks, the models are hyperelastic, anisotropic and fulfill the polyconvexity condition, which implies ellipticity and thus ensures material stability. The first constitutive model is based on a set of polyconvex, anisotropic and objective invariants. The second approach is formulated in terms of the deformation gradient, its cofactor and determinant, uses group symmetrization to fulfill the material symmetry condition, and data augmentation to fulfill objectivity approximately. The extension of the dataset for the data augmentation approach is based on mechanical considerations and does not require additional experimental or simulation data. The models are calibrated with highly challenging simulation data of cubic lattice metamaterials, including finite deformations and lattice instabilities. A moderate amount of calibration data is used, based on deformations which are commonly applied in experimental investigations. While the invariant-based model shows drawbacks for several deformation modes, the model based on the deformation gradient alone is able to reproduce and predict the effective material behavior very well and exhibits excellent generalization capabilities. Thus, in particular the second model presents a highly flexible constitutive modeling approach, that leads to a mathematically well-posed problem.

References

[1] D. Klein, M. Fernández, R. J. Martin, P. Neff and O. Weeger. "Polyconvex anisotropic hyperelasticity with neural networks". In: *Pre-print under review* (2021). arXiv: 2106.14623.

Model order reduction techniques for multiscale fatigue simulations of short fiber reinforced polymers

Jonathan Köbler[1], Nicola Magino[1], Matthias Kabel[1], Heiko Andrä[1], Ralf Müller[2], Matti Schneider[3], Fabian Welschinger[4]

[1]) Fraunhofer ITWM, Department of Flow and Materials Simulation, Germany
jonathan.koebler@itwm.fraunhofer.de
[2]) Technische Universität Kaiserslautern, Institute of Applied Mechanics, Germany
[3]) Karlsruhe Institute of Technology (KIT), Institute of Engineering Mechanics, Germany
[4]) Robert Bosch GmbH, Corporate Sector Research and Advance Engineering, Germany

Short fiber reinforced polymers are of central importance in many industrial applications such as lightweight constructions. The processing of these composite materials by injection molding to components with complex geometries makes them cost-efficient, in particular when produced in large numbers. However, due to the complex microscopic structure of short fiber reinforced polymers their experimental characterization is tedious and time consuming.

To reduce the experimental effort, we present a multiscale database approach [3] which is able to describe the influence of the fiber orientation and loading direction on the macroscopic material behavior. Our database approach is based on the fiber orientation interpolation [3] coupled with model order reduction techniques [1] and full field micro-mechanical simulations [2] on representative volume elements [5].

Combined with a recently developed isotropic non-local fatigue model for the polymer matrix [4], this innovative technique allows us to design a digital twin of short fiber reinforced components with respect to their lifetime under cyclic loading. Simulation results for a window regulator housing demonstrate the efficiency of our scheme for predicting the fatigue behavior of components of industrial complexity.

References

[1] J. C. Michel and P. Suquet. Nonuniform transformation field analysis. *International Journal of Solids and Structures*, 40(25):6937–6955, 2003.

[2] M. Kabel, A. Fink, and M. Schneider. The composite voxel technique for inelastic problems. *Computer Methods in Applied Mechanics and Engineering*, 322:396–418, 2017.

[3] J. Köbler, M. Schneider, F. Ospald, H. Andrä, and R. Müller. Fiber orientation interpolation for the multiscale analysis of short fiber reinforced composite parts. *Computational Mechanics*, 61(6):729–750, 2018.

[4] J. Köbler, N. Magino, H. Andrä, F. Welschinger, R. Müller, and M. Schneider. A computational multi-scale model for the stiffness degradation of short-fiber reinforced plastics subjected to fatigue loading. *Computer Methods in Applied Mechanics and Engineering*, 373:113522, 2021.

[5] M. Schneider. The sequential addition and migration method to generate representative volume elements for the homogenization of short fiber reinforced plastics. *Computational Mechanics*, 59(2):247–263, 2017.

Tumor Control vs. Normal Tissue Complication Probabilities, the Multicriteria Model and Optimization of Radiotherapy

Karl-Heinz Kuefer, Philipp Suess, Katrin Teichert

Fraunhofer Intstitute for Industrial Mathematics ITWM,
Fraunhofer-Platz 1, 67663 Kaiserslautern, Germany,
karl-heinz.kuefer@itwm.fraunhofer.de

Since the early 20th century radiotherapy is one of the three main pillars of cancer therapy - destroying cancerous tissue with high energetic x-rays has been one therapeutic stage for 60 percent of cancer patients worldwide. Since the invention of intensity modulated radiotherapy (IMRT) in the end of the eigthies radiotherapy often replaces surgery at clinical sites where surgery is impossible or too risky.

The major problem of radiotherapy and its planning is the fact that one cannot avoid passing through healthy tissue for physical reasons. So, radiotherapy planning has to balance tumor control probability (TCP), achieved by a tissue dependent higher dose in the target volume, and normal tissue complication probability (NTCP), achieved by keeping doses in organs at risk (OAR) as low as possible. Thus, radiotherapy is inherently a multcriteria optimization problem as finding a good balance of TCP and NTCP is highly indidvidual with regard to tumor characteristics and patient needs.

When we take into account that modern radiotherapy treatment machine allow for tenthousands to hundredthousands of degrees of freedom while simltaneously the dose distribution in the body is controlled in millions of volume elements it is no surprise that simulation and optimization of radiotherapy has belonged to the oldest civil applications of computers reaching back to the early fifties. Mathematically, radiotherapy planning is a nonlinear, genenerally nonconvex, large scale multicriteria optimization problem. Many medical physicists and mathematicians have been engaged in order to simulate and to optimize dose distributions in the relevant parts of the body. Regarding optimization, most often the multiple criteria setup have been scalarized using weight based sums of the objectives. And, the decision process has been based on finding better and more suitbale weights by a time consuming trial and error process of guessing weights, inspecting results and adaptation of weights. With such an approach there is basically no control of optimality and the stopping rule of the process is timeout.

Since the late nineties Fraunhofer ITWM together with German Cancer Research Center, Harvard Medical School, LMU Munich, different hospitals in Germany and the US and later on with commercial companies have adressed this problem by setting up a better decision process that is based on the set of Pareto optimal solutions. After specifying the case with tolerance doses,

curative doses, constraints and its objective functions (5-15 depending on the case) relevant parts of the Pareto surface are approximated based on sparse and adaptively chosen sets of representatives. Algorithmically, modified sandwiching techniques relying on simplices or hyperboxes have beed developed and are used to tackle this in an efficient way. Afterwards, these Pareto solutions are presented to the dosimetrists or the physicians by a navigation engine. This allows the decision makers to surf on the Pareto front in an intuitive way and in real time. This Fraunhofer invention has brought up a game changer in radiotherapy planning: time savings in planning by up to 80 percent and simultaneously finding better treatments for the patient convinced clinical decision makers and commercial companies to invest. Today, world market leader Varian Medical Systems and others distribute radiotherapy planning based on this innovation.

The talk will give a survey on the achievements, the mathematics behind and illustrations of clinical cases. In the end an outlook will show next challenges in radiotherapy planning based on mathematical models.

An Efficient Model Order Reduction Scheme for Dynamic Contact in Linear Elasticity

Diana Manvelyan[1], Bernd Simeon[2], Utz Wever[3]

[1]) Siemens AG
diana.manvelyan@siemens.com
[2]) TU Kaiserslautern
[3]) Siemens AG

We propose an approach for the efficient model order reduction of dynamic contact problems in linear elasticity. Instead of the augmented Lagrangian method that is widely used for mechanical contact problems, we prefer here the Linear Complementarity Programming (LCP) method as basic methodology. It has the advantage of resulting in the much smaller dual problem that is associated with the governing variational principle and that turns out to be beneficial for the model order reduction. Since the shape of the contact zone depends strongly on the acting outer forces, the LCP for the Lagrange multipliers has to be solved in each time step. The model order reduction scheme, on the other hand, is applied to the large linear system for the displacements and computed in advance by means of an Arnoldi process in combination with the Craig-Bampton substructuring technique. In terms of computational effort the reduction scheme is very appealing because the contact constraints are fully satisfied while the reduction acts only on the displacements. As major benefits, the model order reduction preserves the nodes in the contact zone and does not require any snapshot data. In future work we want to address contact problems with non-linear constraints and more complex geometries.

Precontitioning of multiphysics problems using rational approximations

Svetozar Margenov

Institute of Information and Communication Technologies, BAS, Sofia, Bulgaria
margenov@parallel.bas.bg

Multiphysics or multiscale problems often involve coupling at interfaces which are manifolds of lower dimensions, thus giving rise to interface conditions formulated in fractional Sobolev spaces [1]. Consider as a simple example the elliptic problem in Ω in the mixed form

$$\begin{pmatrix} I & -\nabla & T^* \\ \nabla\cdot & 0 & 0 \\ T & 0 & 0 \end{pmatrix} \begin{pmatrix} u \\ p \\ \lambda \end{pmatrix} = \begin{pmatrix} f \\ g \\ h \end{pmatrix},$$

where T is a trace operator on the manifold Γ either within Ω or at its boundary, and the block-diagonal preconditioner $Diag\left((I-\nabla\nabla\cdot)^{-1}, I, (-\Delta)^{1/2}\right)$. The efficient implementation of such preconditioners requires a proper approximation of the inverse of the discrete fractional Laplacian A^s. The spectral decomposition of the matrix A is directly applicable in very limited simplified cases. For this purpose, scalable multigrid methods for discrete fractional Sobolev spaces are developed in [1]. The abstract additive multilevel framework is adapted there. The constructed smoother involves small blocks in the form $A_{k,\nu}^{-s}$. They have a size ν equal to the graph-degree of the corresponding mesh node.

As an alternative, we propose to use the best uniform rational approximation (BURA) method for A^{-s}, $s \in (0,1)$. The aim is to improve the overall computational complexity of the preconditioning algorithm. As correctly noted in [1], a disadvantage of the method introduced in 2018 is that the accuracy depends on the condition number of the matrix A. This drawback is overcome in the improved BURA approximation developed in [2]. It reads as $A^{-s} \approx \lambda_{1,h}^{-s} r_{s,k}(\lambda_{1,h} A^{-1})$, $r_{s,k}$ is the best uniform rational approximation of degree k of z^s on $[0,1]$. The L^2 error $E_{s,k} = O\left(e^{-2\pi\sqrt{ks}}\right)$. Further improvement of the computational efficiency of the BURA methods is presented in [3], where problem-specific model reduction techniques are utilised. Note that the approach discussed is directly applicable to the case of intersecting interfaces, as well as to coupled PDEs defined on domains with different dimensionality.

References

[1] T. Bærland, M. Kuchta, K.-A. Mardal, Multigrid methods for discrete fractional Sobolev spaces, SIAM J. Sci. Comput., 41(2), 2019

[2] S. Harizanov, R. Lazarov, S. Margenov, P. Marinov, J Pasciak, Analysis of numerical methods for spectral fractional elliptic equations based on the best uniform rational approximation, Journal of Computational Physics, 408, 2020

[3] S. Harizanov, N. Kosturski, I. Lirkov, S. Margenov, Y. Vutov, Reduced Multiplicative (BURA-MR) and Additive (BURA-AR) Best Uniform Rational Approximation Methods and Algorithms for Fractional Elliptic Equations, Fractal and Fractional, 5 (6), 2021

On structure-preserving model order and complexity reduction

Nicole Marheineke[1]

[1]) Lehrstuhl Modellierung und Numerik
FB IV - Mathematik, Universität Trier
marheineke@uni-trier.de

In various contexts it has been shown that exact preservation of fundamental structural properties of the problem to be approximated leads to better results in view of stability and accuracy. This talk focuses on the development of structure-preserving and robust approximations for a class of nonlinear flow problems on networks. This class covers, e.g., the Euler equations. The development is guided by energy-based modeling concepts (port-Hamiltonian formalism, theory of Legendre transformation). By combining mixed variational Galerkin approximations with a quadrature-type complexity reduction, the snapshot-based approach yields online-efficient reduced models that guarantee local mass conservation and an energy bound and exhibit an port-Hamiltonian structure. These structural properties are inherited by imposing a few mild compatibilty conditions on the reduction steps. While these conditions are beneficial for the resulting reduced models, they pose a challenge in the training phase, as data optimization problems with constraints have to be solved. The presented model order reduction fulfills an optimality under the compatibility and can be considered as a compatible modification of proper orthogonal decomposition. The complexity reduction leads to a semidefinite program with combinatorial aspects, which is approached by a greedy procedure. Numerical comparisons with non-structure-preserving alternatives from literature underline the advantages of the presented approach. Additional performance improvements can be achieved by a novel extended group finite element method.

Data analytics and optimization in production and logistics

Alexander Martin[1]

[1]) FAU Erlangen-Nürnberg
Department of Data Science
Cauerstr 11, D-91058 Erlangen
alexander.martin@fau.de
and
Fraunhofer Institute for Integrated Circuits
Nordostpark 84, D-90411 Nürnberg
alexander.martin@iis.fraunhofer.de

In this more application-oriented talk we start by giving an overview of methods typically used in the context of data analytics and AI. We will especially focus on applications where the combination of at least two of these methods was essential for the solution of the underlying problem. The topics reach from gas and water network optimization problems, via energy-efficient design of timetables and infrastructures to optimal cash management. We conclude with some lessons learned and a view into future challenges.

(Localized) Model Reduction with Adaptive Enrichment for PDE Constrained Optimization

Mario Ohlberger[1]

[1]) Mathematics Münster, Einsteinstr. 10, D-48149 Münster
mario.ohlberger@uni-muenster.de

Model order reduction is a very active research field that has seen tremendous development in recent years, both from a theoretical and application point of view. A particular promising model reduction approach for parameterized partial differential equations (pPDEs) is the Reduced Basis (RB) Method that relies on the approximation of the solution manifold of pPDEs by low dimensional linear spaces that are spanned from suitably selected particular solutions, called snapshots. While RB methods are meanwhile very well established and analyzed for scalar coercive problems, there are still major challenges for problems with a slow convergence of the Kolmogorov N-width [4]. Particular promising approaches for high dimensional parameter dependence or for multiscale problems are localized model reduction approaches. We refer to [2] for a recent review of such approaches. Based on efficient a posteriori error control and online enrichment, these methods overcome traditional offline/online splitting and are thus particularly well suited for applications in optimization or inverse problems. In this talk we investigate model reduction with adaptive basis enrichment within an Trust Region – RB approach that updates the reduced model during the trust region iteration, cf. [3, 1]. We discuss a posteriori error estimation, convergence of the overall method as well as numerical experiments that demonstrate the efficiency of the approach.

References

[1] Banholzer, S., Keil, T., Mechelli, L., Ohlberger, M., Schindler, F., Volkwein, S.: An adaptive projected newton non-conforming dual approach for trust-region reduced basis approximation of pde-constrained parameter optimization. To appear in Pure Appl. Funct. Anal., 2021+.

[2] Buhr, A., Iapichino, L., Ohlberger, M., Rave, S., Schindler, F., Smetana, K.: Localized model reduction for parameterized problems. P. Benner (ed.) et al., Model order reduction. Volume 2: Snapshot-based methods and algorithms. Berlin: De Gruyter. 245-305 (2021).

[3] Keil, T., Mechelli, L., Ohlberger, M., Schindler, F., Volkwein, S.: A non-conforming dual approach for adaptive trust-region reduced basis approximation of PDE-constrained parameter optimization. ESAIM Math. Model. Numer. Anal. 55(3):1239–1269, 2021.

[4] Ohlberger, M., Rave, S.: Reduced basis methods: Success, limitations and future challenges. Proceedings of the Conference Algoritmy pp. 1–12 (2016).

Generalization Through Controlled Optimization

Rohit Pochampalli[1], Nicolas R. Gauger[2]

Chair for Scientific Computing,
TU Kaiserslautern, Paul-Ehrlich-Strasse, 34-36
67663 Kaiserslautern, Germany
[1]) rohit.pochampalli@scicomp.uni-kl.de
[2]) nicolas.gauger@scicomp.uni-kl.de

Two qualitites that determine effectiveness of machine learning models for real world applications are the generalization ability and robustness with respect to data. The generalization ability of machine learning models is usually considered to be related to model complexity. For models such as deep neural networks, however, the generalization ability does not typically suffer despite having near infinite capacity. Rather, the factors that influence the generalization ability are those that stem from the training of the model, such as early stopping and the batch size used in stochastic mini-batch gradient descent algorithms. A related notion is that of robustness of the model with respect to the data, in the sense that small perturbations in the data result in small perturbations in the model's output. As a rough distinction, sharper minima of the learning problem are less robust compared to flatter ones. In this work we consider the role of such flat minima in the generalization ability of neural networks. In particular a first order optimization algorithm is proposed with line search rules that can control the gradient flow away from steep minima. We present recent results from the investigation of this algorithm on a non-smooth function and also consider a stochastic mini-batch version that could be used to train large scale neural networks.

Combining CFL-like conditions and multirate DAE framework for applications in system simulation software

Michael Kolmbauer[1], Günter Offner[2], Ralf Uwe Pfau[2], Bernhard Pöchtrager[3]

[1]) MathConsult GmbH, Altenberger Str. 69, 4040 Linz, Austria
michael.kolmbauer@mathconsult.co.at
[2]) AVL List GmbH, Hans-List-Platz 1, 8020 Graz, Austria
guenter.offner@avl.com, ralf-uwe.pfau@avl.com
[3]) RICAM, Austrian Academy of Sciences, Altenberger Str. 69, 4040 Linz, Austria
bernhard.poechtrager@ricam.oeaw.ac.at

The importance of system simulation has increased significantly in the automotive industry in recent years. Reasons for this are not just the improved performance of computer systems and the software being used, but also the increasing complexity of the multi-physical systems to be modeled, which are supposed to run both in office and real-time (RT) applications. Modern simulation packages such as AVL CRUISE^{TM}M[1] provide concepts for the automatic generation and stable simulation of dynamic system models. Systems are constructed on a modular basis. Standardized components can be coupled with each other and form physical networks. These in turn can be coupled and form the overall system. For instance, an HEV (hybrid electric vehicle) can be divided into electrical, fluid, gas, mechanical and thermal networks. On the one hand, the overall system can be calculated on a single time step rate (singlerate). On the other hand, the overall system can be decomposed into its physical subnetworks, which are co-simulated with each other at different time scales (multirate). This approach usually leads to a significant simulation speed-up while maintaining sufficient accuracy. Therefore, efficient simulation of each domain as well as of several or even all coupled domains is of high importance.

The mathematical model results from the characteristic equations of the individual network components. These are folded with the underlying network graph satisfying a differential algebraic equation (DAE) which are typically of (differential) index greater 1. Via index reduction and modeling restrictions we obtain models with (differential) index 1. Each physical subsystem as well as the overall system can be solved e.g. by implicit or explicit Runge-Kutta methods. Besides error based adaptive solvers and fixed step solvers, there is also the possibility of a component based step size control using physical based CFL (Courant-Friedrichs-Lewy)-like conditions, which are available for electric, gas and fluid circuits. This results in two main benefits. First, one is not forced to analyse the step sizes and estimate them via trial and error. Second, the step sizes derived from the CFL-like condition allow large steps and guarantees the stability of the method at the same time. In combination with the multirate approach, both provide the necessary ingredients for a stable high performance and possibly real-time capable system simulation.

[1]https://www.avl.com/de/cruise-m

3D image based stochastic micro-structure modelling of foams for simulating elasticity

Claudia Redenbach[1], Sarah Staub[2], Katja Schladitz[2], Anne Jung[3]

[1]) Technische Universität Kaiserslautern, Mathematics Department, Kaiserslautern
redenbach@mathematik.uni-kl.de
[2]) Fraunhofer-Institut für Techno- und Wirtschaftsmathematik, Kaiserslautern
[3])Universität des Saarlandes, Technical Mechanics, Saarbrücken

Random tessellation models from stochastic geometry are powerful tools for studying relations between the microstructure of a cellular material and its mechanical properties. In practice, a tessellation model can be fit to a real microstructure using geometric characteristics which are estimated from 3D image data obtained by micro computed tomography (μCT).

In this work, an open-cell aluminium alloy foam sample with a nominal pore size of 10 ppi and a porosity of 94.2 % is investigated. The analysis is based on a μCT scan of a cubical sample with 40 mm edge length. A Laguerre tessellation model is fit to the reconstructed cell system of the foam. The solid component is then modelled by the dilated edge system of the tessellation. Both circular and triangular cross section shapes are considered, see Figure 1.

In a next step, the effective elastic moduli of the model foams are computed. The simulations are performed in the ElastoDict module of the software GeoDict. The solver is based on the solution of the Lippmann-Schwinger equations for elasticity. Thus, it is very suitable for the computation of effective properties of large microstructured porous structures.

To validate the simulation, a reference simulation is performed on the binarized μCT image of the real foam. The results are in good agreement with the outcome of a compression test of a foam sample.

Simulation of the elastic properties of several variants of the model foam then allows to study the impact of particular modelling parameters on the effective foam behavior.

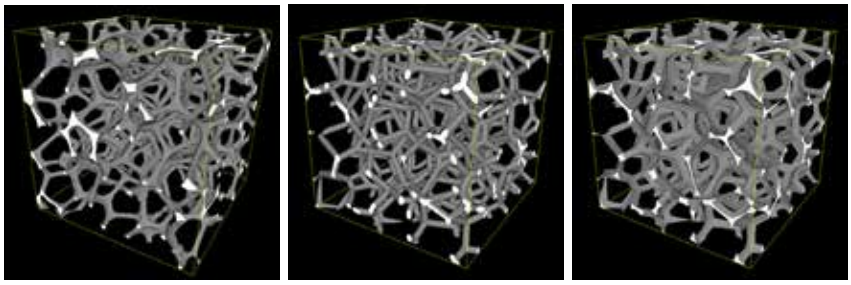


Figure 1: Volume renderings of the CT image of the real foam and of two model foams with cylindrical and triangular strut cross section (from left to right).

Large Deformations of Metal Foams: Dynamic CT Results, Simulations and Modeling

Sebastian Rief[1], Erik Glatt[1], Martina Hümbert[1], Andreas Grießer[1], Wesley De Boever[2], Matthias Kabel[3], Hannes Grimm-Strele[3]

[1]) Math2Market GmbH
info@math2market.de
[2]) Tescan
[3]) Fraunhofer ITWM

Metal foams are used in a wide range of applications, for example in energy dissipation and as lightweight materials. When metal foams are an integral part of a structure, the mechanical characteristics and their response to external load need to be well understood. To facilitate a greater understanding, we have utilized lab-based dynamic computed tomography (CT) provided by Tescan to visualize uninterrupted compression of aluminum metal foams. These results were compared to mechanical simulations of the same samples run with the simulation software GeoDict. The dynamic CT reveals the different modes of deformation, like buckling or bending of struts and collapsing of cells. Moreover, the displacement and deformation of pores can be analyzed and quantified once the scan is imported into the software.

The simulation of the compression up to 35% is possible thanks to the explicit approach of the FFT-based solver FeelMath in GeoDict. By comparing simulation and scan, the simulation can be verified in two ways: First, the load curves show whether the stresses in the foam are similar in simulation and experiment. Second, the different deformation modes observed in the simulation can be compared to the deformation modes in the scan, as well as the evolution of pore shapes with increasing compression. Two samples from the same foam are tested, analyzed, and simulated.

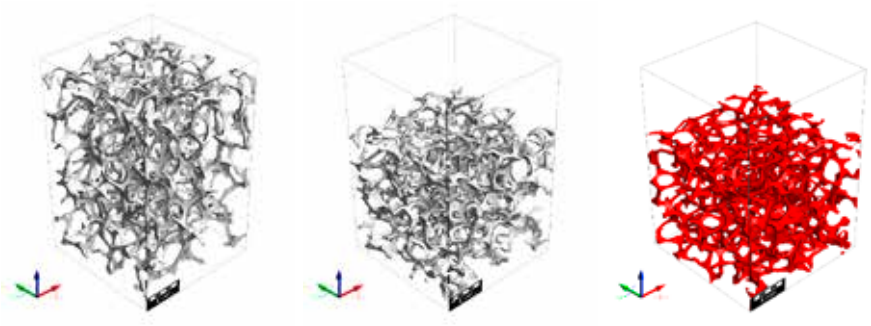


Figure 1: Left: Segmented CT Scan before compression, Middle: Segmented CT scan at 35% compression, Right: Simulation result of compression to 35%

Generating dynamic human motion with optimal control

Michael Roller[1], Staffan Björkenstam[2], Monika Harant[1], Marius Obentheuer[1], Joachim Linn[1]

[1]) Fraunhofer ITWM
michael.roller@itwm.fraunhofer.de
[2]) Fraunhofer Chalmers Center

In industry, there is an increasing demand on simulating the dynamic motion of a human and its interaction with the environment. Thereby industry is interested on the ergonomic assessment of the movement, for example when assembling parts, moving heavy objects, driving a car or standing in a autonomous driving train. For this sake, the simulation should produce human like motion with correct inner forces, even if there is only a simple task description like, move part from A to B or take over steering wheel. Today, industry is either using static human models for such simulation cases and combine static posture to a dynamic motion or generate the dynamic human motion by motion capturing of real human. Nevertheless, in static simulation it is impossible to inertia effects and motion capturing is very cost and time demanding because physical prototypes are needed. To create a model, which fulfills the requirements above, optimal control of a biomechanical multibody mode is used.

In this approach, the skeletal system of the human is modeled as a multibody system (MBS). The equations of motion of the MBS are a system of differential algebraic equations. To control the biomechanical system in a more realistic way muscles have to be included into the simulation scenario. We restrict ourselves to a string type Hill-model, where the active contractile element creates a pulling force depending on the activation, the length and the contraction velocity of the muscle. A muscle is connected to the MBS through at least two body points.

To generate human like motion with a biomechanical MBS, an optimal control approach is used, where the control signals are the activations of the muscles. Therefore, a time continuous optimization problem arises, where the equation of motion and also the tasks are included as constraints. The objective function can be used to generate trajectories with a given characteristic, like minimal control effort, minimal kinetic energy or minimal execution time. The continuous optimal control problem is approximated with the so called DMOCC (discrete mechanics and optimal control for constrained systems) approach, where a variational integrator is used to discretize the equation of motion. Hence, a finite dimensional nonlinear optimization problem with nonlinear constraints arises, which is solved with an interior point method. With such a modeling approach, it is possible to generate human-like motion for typical working procedures, sport movements, passive and active driving scenarios.

State-Time Formulation to Reduce the Temporal Dimension in Design Optimization

Ward Rottiers[1,2], Frank Naets[1,2], Wim Desmet[1,2]

[1] Department of Mechanical Engineering, KU Leuven, Belgium
ward.rottiers@kuleuven.be
[2] DMMS Lab, Flanders Make, Leuven, Belgium

Depending on the analysis, the model describing an industrial asset can vary from a low-dimensional lumped parameter model (typically $n_s < 10^2$) to a high-dimensional distributed parameter model (typically $n_s \in [10^4 - 10^8]$). Early-stage design optimization is typically performed on low-dimensional, nonlinear models to compute optimal parameters $\mathbf{p}^*$ in order to compare multiple topologies or to pass on to a next design stage. Objective functions describing dynamic behavior over a wide range of operational conditions require a transient analysis over a long simulated time, resulting in a high temporal dimension (typically $n_t \in [10^6 - 10^9] \gg n_s$).

Classical model reduction methods are well suited to reduce high-dimensional full order model (FOM) equations, resulting in often less numerically stiff reduced order model (ROM) equations. Hence, the temporal dimension is indirectly influenced only if a significant state/spatial dimension reduction is achieved.

In order to reduce the computational cost of early-stage design optimization with an objective consisting of a transient analysis, a temporal dimension reduction method is developed based on the work of Choi and Carlberg [1]. "The temporal reduction considers the time-discretized algebraic system

$$\mathbf{D}\chi = \mathbf{s}\left(\chi, \mathbf{x}_0, \mathbf{p}\right), \tag{1}$$

with the state-time vector $\chi = \left\{\mathbf{x}^T[1], ..., \mathbf{x}^T[n_t]\right\}^T \in \mathbb{R}^{(n_s.n_t)}$, the initial condition $\mathbf{x}_0 \in \mathbb{R}^{n_s}$ and the state difference $\mathbf{D} \in \mathbb{R}^{n_s.n_t \times n_s.n_t}$ and system specific $\mathbf{s} \in \mathbb{R}^{n_s.n_t}$ contribution of the time discretization. Equation (1) is reduced via a Galerkin projection with a basis computed via a higher-order singular value decomposition of training data. The nonlinear term $\mathbf{s}\left(\chi, \mathbf{x}_0, \mathbf{p}\right)$ is furthermore hyper-reduced via an adapted DEIM approach. As a result, the evaluation of the reduced algebraic system or state-time ROM (STROM) requires only the (parallel) evaluation of the state propagation at certain time steps [2]."

This work discusses the error analysis of the temporal dimension reduction, adaptations to the DEIM sampling and the temporally reduced evaluation during optimization. The optimization is performed on a longitudinal and lateral vehicle dynamics model including tire behavior.

[1] Y. Choi and K. Carlberg. Space–Time Least-Squares Petrov–Galerkin Projection for Nonlinear Model Reduction. *SIAM Journal on Scientific Computing*, 41(1):A26-58, 2019.

[2] W. Rottiers, F. Naets and W. Desmet. Temporal dimension reduction via parametric state–time formulation.. *MORTech 2019-5th international Workshop; Reduced Basis, POD and PGD Model Reduction Techniques.*, 2019.

The binary knapsack problem with qualitative levels

Luca E. Schäfer[1], Tobias Dietz[1], Maria Barbati[2], Jose Rui Figueira[3], Salvatore Greco[2,4], Stefan Ruzika[1]

[1]) Department of Mathematics, Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany
arthur.author@correspondence.email.com
[2]) Department of Economics and Business, University of Catania, Catania 95129, Italy
[3]) CEG-IST, Instituto Superior Tcnico, Universidade de Lisboa, 1049001 Lisboa, Portugal
[4]) Portsmouth Business School, Centre of Operations Research and Logistics (CORL), University of Portsmouth, PO1 3DE Portsmouth, United Kingdom

A variant of the classical knapsack problem is considered in which each item is associated with an integer weight and a qualitative level instead of a numeric profit value.

By using reasonable numerical representations for the different qualitative levels, we define a dominance relation over the feasible subsets of the given item set and show that this relation defines a preorder. More specifically, a numerical representation is said to be reasonable, if it preserves the order of the qualitative levels, i.e., the higher the rank of the qualitative level, the higher the corresponding numeric value. Based on this dominance relation, we define the concepts of qualitative non-dominance and efficiency, which are in line with the classical dominance concepts in multiobjective optimization.

By introducing rank cardinality vectors that count the number of items with respect to each qualitative level in an item set, we come up – as our main result – with a simple, yet powerful optimality criterion that can decide on the dominance relation between two different item sets in constant time without even considering numerical representations.

Moreover, we prove that the number of non-dominated rank cardinality vectors is polynomially bounded for a fixed number of qualitative levels. Based on that, we propose a dynamic programming algorithm that is quite similar to the dynamic program for the classical knapsack problem to compute the entire set of non-dominated rank cardinality vectors in pseudopolynomial time.

Additionally, by defining two different lexicographical orders, we state two greedy algorithms, which efficiently compute a single non-dominated solution in polynomial time.

Finally, we point out several interesting connections of the qualitative knapsack problem to multiobjective optimization.

A General Framework for Machine Learning based Optimization Under Uncertainty and Inverse Problems

Philipp A. Guth[1], Claudia Schillings[1] and Simon Weissmann[2]

[1]) Institute for Mathematics, University of Mannheim
c.schillings@uni-mannheim.de
[2]) Interdisciplinary Center for Scientific Computing, University of Heidelberg

Approaches to decision making and learning mainly rely on optimization techniques to achieve "best" values for parameters and decision variables. In most practical settings, however, the optimization takes place in the presence of uncertainty about model correctness, data relevance, and numerous other factors that influence the resulting solutions. For complex processes modeled by nonlinear ordinary and partial differential equations, the incorporation of these uncertainties typically results in high or even infinite dimensional problems in terms of the uncertain parameters as well as the optimization variables, which in many cases are not solvable with current state of the art methods. One promising potential remedy to this issue lies in the approximation of the forward problems using novel techniques arising in uncertainty quantification and machine learning.

We propose in this talk a general framework for machine learning based optimization under uncertainty and inverse problems. Our approach replaces the complex forward model by a surrogate, e.g. a neural network, which is learned simultaneously in a one-shot sense when estimating the unknown parameters from data or solving the optimal control problem. By establishing a link to the Bayesian approach, an algorithmic framework is developed which ensures the feasibility of the parameter estimate / control w.r. to the forward model.

A machine-learning-based approach for finding recovery-robust timetables

Matthias Müller-Hannemann[1], Ralf Rückert[1], Alexander Schiewe[2], Anita Schöbel[2,3]

[1]) Martin-Luther-Universität Halle-Wittenberg
[2]) TU Kaiserslautern
[3]) Fraunhofer ITWM, Kaiserslautern

Optimizing timetables in public transport planning is a challenging process. There are several possible criteria to evaluate. Here, we focus on two aspects: The travel time of the passengers and the robustness against delays. In this talk, we consider the recovery robustness of a timetable, i.e., the performance of a timetable not in the nominal case but in the case of delays after applying a given recovery or disposition strategy. Unfortunately, a passenger-based evaluation of robustness for timetables is very time consuming since many different possible delay scenarios need to be simulated realistically. Using this criterion as a base for optimization is therefore challenging.

In this talk we present an alternative approach to evaluating the robustness of a timetable while still allowing to use this measurement in optimization procedures. For this we train a machine-learned oracle on approximating the recovery robustness of a timetable and a corresponding vehicle schedule. For this, we define key features of a given solution, which can be used as an input for a neural network and provide an estimated recovery robustness value with high accuracy.

This oracle is used with two different algorithmic approaches, a local search framework as well as a genetic algorithm approach. We discuss several possible neighborhood definitions for the local search as well as different approaches for the genetic algorithm. For these iterative approaches we consider both objectives: Improving the robustness of starting solutions while keeping the passenger travel time at an acceptable level.

We evaluate both appraoches on artificial and close-to real-world benchmark datasets. We see that initial solutions can be improved w.r.t. travel time of the passengers and robustness, i.e., new competitive, non-dominated solutions can be found. Comparing this new solution approach to other state-of-the-art timetabling methods, the set of non-dominated solutions can be extended drastically, allowing for better and different trade-offs between travel time and recovery robustness.

On using reduced order models in adaptive data-augmented training of machine learning models for reactive flow

Pavel Gavrilenko[3], Bernard Haasdonk[2], Oleg Iliev[3], Mario Ohlberger[1], Felix Schindler[1], Pavel Toktaliev[3], Tizian Wenzel[2], Maha Youssef[2]

[1]) Mathematics Münster, Westfälische Wilhelms-Universität Münster, Einsteinstr. 62, 48149 Münster {mario.ohlberger,felix.schindler}@uni-muenster.de
[2]) Institute of Applied Analysis and Numerical Simulation, Pfaffenwaldring 57, 70569 Stuttgart
{haasdonk,tizian.wenzel,maha.youssef-ismail}@mathematik.uni-stuttgart.de
[3] Fraunhofer-Institut für Techno und Wirtschaftsmathematik, Fraunhofer-Platz 1, 67663 Kaiserslautern
{oleg.iliev,pavel.gavrilenko,pavel.toktaliev}@itwm.fraunhofer.de

Extending [3], we present an adaptive approach for the use of simulated data from full order discretization as well as projection-based Reduced Basis reduced order models [1] for the training of machine learning approaches, in particular Kernel Methods [2], in order to achieve fast, reliable predictive models for the chemical conversion rate in reactive flows with varying transport regimes within the BMBF-funded project on "Maschinelles Lernen und Modelordnungs - Reduktion zur Vorhersage der Effizienz katalytischer Filter".

References

[1] Benner, P., Cohen, A., Ohlberger, M., Willcox, K. (eds.): Model reduction and approximation: theory and algorithms, Computational Science & Engineering, vol. 15. SIAM, Philadelphia, PA (2017)

[2] Santin, G., Haasdonk, B.: Kernel methods for surrogate modeling. ArXiv 1907.10556 (2019)

[3] Gavrilenko, P., Haasdonk, B., Iliev, O., Ohlberger, M., Schindler, F., Toktaliev, P., Wenzel, T., Youssef, M.: A full order, reduced order and machine learning model pipeline for efficient prediction of reactive flows. Contributed to the 13th International Conference on Large-Scale Scientific Computations (LSSC 2021), Sozopol, Bulgaria. ArXiv 2104.02800 (2021)

Online and Offline Calibration of Digital Twins in the Smart Assembly 4.0 Framework

Anders Sjöberg[1,3], Magnus Önnheim[1,3], Otto Frost[1,3], Constantin Cronrath[2], Emil Gustafsson[1,3], Bengt Lennartson[2], and Mats Jirstrand[1,3]

[1]Fraunhofer-Chalmers Centre [2]Chalmers University of Technology
[3]Fraunhofer Center for Machine Learning

The overarching objective of the project *Smart Assembly 4.0* has been to address research challenges related to the realization of the autonomous, self-optimizing robotized assembly factory, which maximizes quality and throughput, maintaining flexibility and reducing cost, by a sensing, thinking and acting strategy [1].

A specific goal has been to develop a digital twin of a sheet metal welding production cell in an assembly line, including the modeling of the geometric path planning of the robotics, individual part variation as measured by sensors before welding, physical models for the deformation of assemblies during welding, feedback control, and data driven process improvement. Detailed modeling of the end-to-end assembly process has shown promising results [2, 3].

However, an end-to-end digital twin necessarily consists of many interacting parts. Thus, *calibration* of the digital twin to reality becomes increasingly important, as miscalibration of interacting components may nullify any gains.

We view the family of possible digital twins as a family of functions $\{Q(x, u; \theta\}$, where x denotes an individual assembly to be manufactured, u the controllable parameters, θ parameters to be calibrated, and Q a mapping from inputs and parameters to final assembly quality, as provided by the digital twin.

We view the calibration as a system identification task, and evaluate two approaches. The *offline* or batch mode approach, where a significant number of assemblies are processed and identification is performed by global optimization of the discrepancy between Q and observed assemblies. We show that this simple approach can handle significant errors in initial calibration. The *online* approach considers θ as the state of an unscented Kalman filter [4], for which Q becomes the (non-linear) measurement function, and we show that this approach can track a time-varying ground truth θ_t^*.

We further note that the controllability of the parameters u present an exploration/exploitation trade-off, in the sense that u can be optimized for next-assembly quality or for ease of identification. We propose and evaluate an surrogate model approach for balancing this exploration/exploitation trade-off, and show that, in the evaluated scenarios, an approach favouring exploration significantly outperforms exploitation-focused approaches, as well as naive baselines, in terms of average final quality over many assemblies. However, this comes at the cost of significant computational burden.

Acknowledgements This work has been funded by the Swedish Foundation for Strategic Research (Grant no RIT15-0025) and also been carried out in the Fraunhofer Cluster of Excellence *Cognitive Internet Technologies*.

References

[1] Rikard Söderberg, Kristina Wärmefjord, Johan S Carlson, and Lars Lindkvist. Toward a digital twin for real-time geometry assurance in individualized production. *CIRP Annals*, 66(1):137–140, 2017.

[2] Abolfazl Rezaei Aderiani, Kristina Wärmefjord, Rikard Söderberg, and Lars Lindkvist. Individualizing locator adjustments of assembly fixtures using a digital twin. *Journal of Computing and Information Science in Engineering*, 19(4), 2019.

[3] Constantin Cronrath, Abolfazl R Aderiani, and Bengt Lennartson. Enhancing digital twins through reinforcement learning. In *2019 IEEE 15th International Conference on Automation Science and Engineering (CASE)*, pages 293–298. IEEE, 2019.

[4] Eric A Wan, Rudolph Van Der Merwe, and Simon Haykin. The unscented Kalman filter. *Kalman filtering and neural networks*, 5(2007):221–280, 2001.

An efficient real-time reconstructor for Extremely Large Telescopes

Bernadett Stadler[1], Ronny Ramlau[2]

[1]) Industrial Mathematics Institute, Johannes Kepler University Linz, Austria
bernadett.stadler@indmath.uni-linz.ac.at
[2]) Industrial Mathematics Institute, Johannes Kepler University Linz, Austria

Astronomical imaging with ground-based telescopes suffers from quickly varying optical distortions, which cause blurring and loss of contrast. These optical distortions are induced by turbulences in the earth's atmosphere. Since the contrast and sharpness of images are essential for astronomical observations, a method that compensates for these aberrations is required. This technique is called Adaptive Optics (AO). It utilizes a combination of wavefront sensors, that measure the deformations of wavefronts emitted by guide stars, and deformable mirrors to correct for them. Classical AO systems, using only one guide star, achieve high image quality only near to this guide star. Since there are not enough bright guide stars available, AO systems that achieve a good correction over a large field have been developed. These systems involve a tomographic estimation of the 3D atmospheric wavefront disturbance. Mathematically, the reconstruction of turbulent layers in the atmosphere is severely ill-posed, hence, limits the achievable solution accuracy. Moreover, the reconstruction has to be performed in real-time at a few hundred to thousand Hertz frame rates. This leads to a computational challenge, especially for the AO systems of future Extremely Large Telescopes (ELTs) with a primary mirror up to 40 m.

In this talk we present a wavelet based, iterative method called augmented Finite Element Wavelet Hybrid Algorithm (augmented FEWHA) for solving the atmospheric tomography problem. The key feature of the algorithm is the matrix-free representation of the underlying operators, which leads to a significant reduction in the computational load and memory. Moreover, the method is highly parallelizable. A crucial indicator for the run-time of iterative solvers is the number of iterations. Within augmented FEWHA an augmented Krylov subspace method is utilized in order to reduce the number of Conjugate Gradient iterations. We present an efficient, parallel implementation of the algorithm on a multi-core CPU and a GPU. Moreover, we study the performance of the algorithm in terms of quality and run-time via numerical simulations for ELT-sized test configurations.

A multi-scale model hierarchy for material flow on conveyor belts

Jennifer Weissen[1]

[1]) University of Mannheim
jennifer.weissen@uni-mannheim.de

Virtual commissioning, where the real system is replaced by a digital twin to run tests in interaction with the real control system, enables early testing of the interaction between plant layout and control system. We investigate manufacturing systems with high material flow. The manufacturing system is depicted by a hierarchy of digital twins which use different simulation techniques. Close interaction of different simulations levels enables efficient simulation, validation and optimization.

On the higher level, the digital twin is represented by an engineering simulation in three space dimensions. On the lower level, a partial differential equation (PDE) in two space dimensions enables simulation with short and deterministic calculation time. Our macroscopic model based on a hyperbolic PDE is a well-established approach for the material flow simulation. Until recently, macroscopic models have been exclusively used for the simulation of cylindrical cargo. We show the application of the macroscopic model on cuboid cargo as a new simulation approach for parcel logistics. An experimental setup especially designed for the validation of the considered macroscopic model for cuboid cargo bulk flow on a conveyor belt is presented. We adapt selected model parameters to cover the new situation and compare our simulation results with the microscopic engineering simulation. Furthermore, the finite volume discretization of the macroscopic model allows to efficiently control the conveyor belt velocity. We present numerical results for the optimal controls that are validated using the microscopic simulation.