BOOK OF ABSTRACTS

Conference on

DATA AND PHYSICS-BASED MODELLING, SIMULATION AND OPTIMIZATION IN INDUSTRIAL APPLICATIONS

9-11 October 2024
Széchenyi István University, Győr, Hungary

version 27.09.2024

CONTENT

ABOUT THE CONFERENCE

The traditional physics-based and the more recent data-based modelling, simulation and optimization (MSO) are key technologies of industry and societal applications.

The conference provides researchers and users in academia and industry with an opportunity to present their

- use cases of the MSO-technology,

- recent computational solutions, including HPC-solutions for industrial problems,

- industrial challenges that could be solved by the MSO technology.

The conference is scientifically supported and announced by the collaboration of the national industrial mathematical networks of Hungary, Austria, Croatia and Slovenia, namely HU-MATHS-IN, IMNA, CRO-MATH-IN and SL-MATHS-IN. These networks are active members of the European Industrial Mathematics Network, EU-MATHS-IN.

Research and innovation projects, e.g. the HiDALGO2 Centre of Excellence of EuroHPC JU, the CREATOR project of DFG and FWF will be present to show their competencies.

Highlighted themes of the conference:

- electric machines and drives,

- societal challenges, e.g. air pollution, cancer,

- multibody simulations in industry: manufacturing,

- healthcare, e.g. genomics, medical image processing,

- HPC in industry.

Poster session and a special session on recruiting partners for European proposals (MSCA, Horizon Europe, etc.) will serve the communication and effective networking.

Publication: special issue of the journal ETNA (Electronic Transactions on Numerical Analysis).

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TENTATIVE PROGRAM OVERVIEW

Conference on

DATA AND PHYSICS-BASED MODELLING, SIMULATION AND OPTIMIZATION IN INDUSTRIAL APPLICATIONS

9-11 October 2024
Széchenyi István University, Győr, Hungary

E-mobility
Healthcare
Mechanical engineering
Acoustics
Optics, Telecommunication
Computational methods for applications
Transportation

9 October			Name	Affiliation	Title
12:00	00:10	**Opening**			
12:10	00:40	keynote	Számszi, István	Robert Bosch Kft., Budapest	Innovation and competitive advantage: The new paradigm for the collaboration between the academy and the industry
12:50	00:40	keynote	De Gersem, Herbert	TU Darmstadt	TBA
13:30	00:15	**Break**			
13:45	00:30	invited	Horváth, Csongor	Robert Bosch Kft., Budapest	Current and future challenges of mobility
14:15	00:30	invited	Kolmbauer, Michael	RICAM, and MathConsult Gmbh, Linz	Using Functional Mock-Up Units for Multi-Physical System Simulation in Electric Vehicle Development
14:45	00:20	contributed	Cherrière, Théodore	RICAM, Linz	General multi-material topology optimization framework to design innovative electrical machine
15:05	00:15	**Break**			
15:20	00:40	keynote	Silber, Siegfried	Linz Center of Mechatronics, Linz	Parametric Optimization of Electric Machines
16:00	00:30	invited	Vajsz, Tibor	Robert Bosch Kft., Budapest	Reluctance motor drives: an opportunity to a more sustainable electric transportation
16:30	00:20	contributed	Paiss, Vilmos	Robert Bosch Kft., Budapest	A novel motor model for synchronous reluctance machines of electric vehicles
16:50	00:15	**Break**			
17:05	00:40	keynote	Curk, Jurij	Elektro Ljubljana, Ljubljana	How far can we reasonably push distribution grid operation?
17:45	00:20	contributed	Liljegren-Sailer, Björn	RICAM, and MathConsult Gmbh, Linz	Structure-preserving model reduction of network systems
18:05	00:20	contributed	Kovács, Richárd	Robert Bosch Kft., Budapest	Torque calculation methods for synchronous reluctance machines of e-mobility
18:25	00:20	contributed	Krenn, Nepomuk	RICAM, Linz	Electro-thermal topology optimization of an electric machine
18:45	00:10	**Summary of Day 1**			
18:55	00:20	**Walk to Reception venue (Széchenyi square)**			
19:15	00:30	**Jedlik memory room, first electric motor**			
19:45	01:30	**Reception, in Apátúr house**			
21:15		**End of Day 1**			

10 October			Name	Affiliation	Title
08:30	00:40	keynote	Muha, Boris	U. Zagreb	A computational algorithm to study bioartifcial pancreas scaffold architecture design
09:10	00:30	invited	Petras, Argyrios	RICAM, Linz	Computational methods for cardiac catheter ablation procedures
09:40	00:20	contributed	Hackl, Simon	JKU Linz	Sound Speed and Layer Adapted Focusing Methods in Medical Ultrasound
10:00	00:20	contributed	Huidong Yang	U Vienna	Optimizing data fitting in ultrasound simulations: Exploring linear and nonlinear models
10:20	00:15	**Break**			
10:35	00:30	invited	Röst, Gergely	University of Szeged	TBA
11:05	00:20	contributed	Harangi, Balázs	University of Debrecen	Deep learning-based ensemble system for cytological screening system
11:25	00:20	contributed	Kovács, Péter	Eötvös Loránd University, Budapest	Interpretable representation learning by means of variable projections
11:45	00:20	contributed	Bognár, Gergő	Eötvös Loránd University, Budapest	Applications of deep unfolding in signal processing
12:05	01:00	**Lunch**			
13:05	00:30	invited	Kouri, Alexandria and Pintér, Lajos	SZBK-DeltaBio 2000 Kft.	Machine learning driven genetic variant annotation through HPC
13:35	00:20	contributed	Gordos, Ambrus	VRG Therapeutics Kft.	AI-Driven protein design for next-generation therapeutics
13:55	00:20	contributed	Ligeti, Balázs	Pázmány Péter Catholic University, Budapest	ProkBERT: genomic language models for understanding the microbiome
14:15	00:05	**Break**			
14:20	00:20	invited	Ódor, Géza	HUN-REN Centre for Energy Research	Modelling synchronization phenomena in brain and power-grid networks
14:40	00:30	contributed	Balogh, András	Eötvös Loránd University, Budapest	Ab initio simulations of two-dimensional materials: investigating grain boundaries and HPC architecture performance
15:10	00:30	contributed	Környei, László and Bakosi, József	Széchenyi István University, Győr	TBA
15:40	00:15	**Break**			
15:55	00:30	invited	Felhős, Dávid, and Ady, László	Kármán Next Kft, Budapest	TBA
16:25	00:30	invited	Grubisic, Luka	U. Zagreb	TBA
16:55	00:20	contributed	Sandric, Nikola	U. Zagreb	TBA
17:15	00:20	contributed	Lorenz, Norbert	RICAM, and MathConsult Gmbh, Linz	Thermal Analysis of Hydrodynamic Lubricated Journal Bearings in Automotive and Industrial Applications
17:35	00:20	contributed	Haslinger, Josef	RICAM, and MathConsult Gmbh, Linz	A frequency domain solution for automotive transmission systems
17:55	00:15	**Break**			
18:10	00:20	contributed	Ramlau, Ronny	JKU and RICAM, Linz	Big Data analysis of astronomic telescopes
18:30	00:20	contributed	Stadler, Bernadett	RICAM, and MathConsult Gmbh, Linz	Adaptive Optics simulations for ground-to-satellite communication
18:50	00:10	**Summary of Day 2**			
19:00	00:20	**Walk to the Conference Dinner venue (University Concert Hall - former Synagogue)**			
19:20	02:00	**Conference Dinner**			
21:20		**End of Day 2**			

11 October			Name	Affiliation	Title
08:30	00:40	keynote	Feszty, Dániel	Audi Hungaria, and Széchenyi István University, Győr	Methodology development for simulating mid-frequency vehicle interior noise
09:10	00:40	keynote	TBA		
09:50	00:20	contributed	Esat, Topbas	Audi Hungaria, Győr	Overview and challenges of simulating vehicle interior noise
10:10	00:20	contributed	Constans, Mátyás	Széchenyi István University, Győr	TBA
10:30	00:20	contributed	Izsák, Ferenc	Eötvös Loránd University, Budapest	Efficient room acoustic simulations
10:50	00:15	**Break**			
11:05	00:40	keynote	Egger, Herbert	JKU and RICAM, Linz	TBA
11:45	00:20	contributed	Lohász, Máté	MVM EGI	Air flow simulation of large scale forced draught cooling cells for power plant
12:05	00:20	contributed	Gáspár, Csaba	Széchenyi István University, Győr	Application of a localized Method of Fundamental Solutions to inhomogeneous elliptic problems
12:25	00:20	contributed	Bauer, Klaus-Dieter	RICAM, and MathConsult Gmbh, Linz	Efficient Unbalance Variation on Condensed FE Models
12:45	00:20	contributed	Köthe, Christian	TU Graz	Space-time least-squares FEM for convection-diffusion problems
13:05	00:15	**Break**			
13:20	00:20	contributed	Békési, József	University of Szeged	Automatic planning of vehicle and driver schedules for public transportation: a case study
13:40	00:20	contributed	Dávid, Balázs	InnoRenew Coe, U Primorska, Koper	Mapping and Analysis of Wood Waste Generation, Collection and Handling
14:00	00:10	**Closing**			
14:10	01:00	**Lunch**			
15:10		**End of the conference**			

ABSTRACTS

Ab Initio Simulations of Two-Dimensional Materials: Investigating Grain Boundaries and HPC Architecture Performance

András Balogh, László Oroszlány

Two-dimensional (2D) materials hold significant promise for next-generation electronic, mechanical, and magnetic applications due to their unique physical properties. However, grain boundaries, an inherent structural feature in 2D materials, play a critical role in shaping these properties and present challenges in both understanding and industrial application. In this work, we present ab initio simulations that explore the influence of grain boundaries on the electronic properties of 2D materials. Our approach leverages high-performance computing (HPC) to conduct these simulations across a variety of architectures, offering a comparative analysis of computational performance and efficiency. The results highlight key differences in scalability and resource utilization, providing insights into the optimal use of HPC for material simulation and design. This study contributes to advancing the understanding of 2D materials and supports the development of computational methods for industrial applications in fields such as nanotechnology and materials science.

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Efficient Unbalance Variation on Condensed FE Models

Klaus-Dieter Bauer, Günter Offner

In industrial power train simulations finite element models are reduced to condensed models with a lower number of degrees of freedom to achieve viable simulation times. In this process reduced stiffness, damping and mass matrices are calculated, as well as various inertia invariants needed for calculating inertia forces acting on the nodes of the reduced body in a floating-frame-of-reference formulation without knowledge of the full geometry of the original FE model.

This process is typically computationally expensive and, in practice, typically involves a series of independent software tools to produce the modified models and perform the simulations. Performing parameter studies over the unbalance properties of a body is therefore hampered by the needed manual and computational effort for preparing each variation of the model.

We discuss a method of applying small modifications to the mass distribution of bodies \emph{after} condensation by rigidly attaching points of positive or negative mass to existing nodes of the condensed FE model, that enables updating the condensed properties without knowledge of the full FE model, allowing (a) efficient variation of the unbalance properties without costly recondensation from the full FE model and (b) automated application of the modification directly in the simulation kernel instead of a largely manual multi-software workflow.

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Automatic Planning Of Vehicle And Driver Schedules For Public Transportation: A Case Study

József Békési, Viktor Árgilán, Gábor Galambos, Imre Papp

Operational costs represent a large proportion of the costs of public transport service companies. These costs -- as main components -- include fleet purchase costs, vehicle fuel and maintenance costs, and driver fees. In the past decades using decision support systems the considered models applied complete solutions of both optimization tasks for the public transportation companies.

Vehicle and driver scheduling in public transport can be very complex. In theory, we are generally looking for a global optimum that minimizes both vehicle-related tasks and driver scheduling costs. These two types of costs affect each other, so it is usually the best way to handle the tasks together.

To solve this problem a so called combined vehicle and driver scheduling mathematical optimization models are used. In this model, the optimal schedule can be calculated as a solution of an integer programming problem.

For the driver part the best known technology is the so-called Generate and Select (GaS) method. In the first phase a large number of regular shifts are generated. In the selection phase, a subset of them that minimizes the cost and covers the trips is chosen.

In their paper Békési and Nagy presented how the methods used in the literature were adapted to develop a decision support system for the Budapest Transport Corporation. The aim of this project was to automatically calculate optimal or approximately optimal vehicle and driver schedules for a given list of trips based on the master data and the company specific requirements and parameters in compliance with labor regulations.

This talk overviews how the complete integration was implemented and what kind of specific developments were necessary to take into account all the practical requirements of the company.

Reference:

Békési, J., Nagy, A. (2020). Combined Vehicle and Driver Scheduling with Fuel Consumption and Parking Constraints: a Case Study. {\it Acta Polytechnica Hungarica}, 17(7): 45--65.\

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Applications of Deep Unfolding in Signal Processing

Gergő Bognár, Sándor Fridli

Model-based machine learning combines traditional model-driven methods with machine and deep learning, offering the direct incorporation of mathematical, physical, or statistical domain knowledge into the network architecture. Model-based machine learning provides compact models, optimized representation learning, and also better computational properties compared to general-purpose black-box deep learning approaches. Since the model-based part of the architecture is constructed from a real model, the system parameters usually have explainable interpretation. This leads towards explainable AI, that is especially important in certain application fields, like in the health care sector.

In this talk, we overview the deep unfolding paradigm of model-based neural networks, including the computational background, the mathematical models for encoding domain knowledge, and the relation with classical feature extraction techniques and neural networks (like variable projections, variable projection networks, and recurrent neural networks). We present applications in biomedical signal processing and telecommunications: ECG heartbeat classification for arrhythmia detection, and data estimation in the physical layer of wireless communication systems.

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General multi-material topology optimization framework to design innovative electrical machines

Théodore Cherrière, Peter Gangl, Nepomuk Krenn

Topology optimization's significant promise is to efficiently provide innovative solutions free from initial bias from human choice and bias. Therefore, topology optimization has become increasingly popular in designing electrical actuators. However, such a methodology has to consider multiple materials to hold this promise. The well-used density-based approaches fail to provide meaningful structures when considering several source terms of different natures. This presentation aims to provide a general framework relying on material interpolations based on generalized barycentric coordinates, which can handle such sophisticated optimization problems. Because the proposed approach still requires arbitrary hyper-parameters selected by experts (interpolation domain, material placement), a further extension to simplex interpolation that drastically reduces the number of hyperparameters will be presented. The approaches were successfully applied to the topology optimization of a hybrid-flux rotor pole from an electric vehicle traction machine.

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Mapping and Analysis of Wood Waste Generation, Collection and Handling

Balázs Dávid, Nikola Kovačević

Sustainability has become an extensively discussed topic over the past years, and efficient management and reuse of waste can contribute to this substantially. Wood waste is particularly important in this regard due to its reusable nature. Transforming discarded wood into valuable resources through recycling provides environmental and economic benefits by reducing landfilled waste and contributing to a circular economy. Efficient management of waste depends on both the employed technologies and the effectiveness of the underlying logistics network.

The primary objective of this research is to develop a comprehensive simulation model that studies the generation, collection, and handling of various types of wood waste in Slovenia. Through analyzing available statistical waste data, the study aims to map and evaluate the material flows and transformations of wood waste and create an abstract representation of the underlying material flow network. Based on the above findings, a simulation model will be developed that incorporates spatial analysis to understand the distribution and efficiency of waste collection networks across different regions and years. Additionally, the model will facilitate the comparison of different waste management strategies, enabling the identification of optimal practices for enhancing resource recovery and reducing environmental impact. This study presents the initial challenges of analyzing this statistical data and introduces a discrete event simulation model that is built to incorporate these preliminary observations.

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Application of a localized Method of Fundamental Solutions to inhomogeneous elliptic problems

Csaba Gáspár

Many engineering problems (e.g. thermal, electrical processes, seepage hydraulics etc.) are described by elliptic partial differential equations. At present, the most popular solution technique of such equations is the finite element method. However, it requires defining a proper set of elements, which is often a sophisticated and time-consuming task. In contrast to this, meshless methods require neither domain nor boundary mesh or grid structure. Such a technique is the Method of Fundamental Solutions (MFS), which approximates the exact solution by a linear combination of the relevant fundamental solution shifted to some predefined source points. By enforcing the applied boundary conditions, this results in a linear system of equations for the unknown coefficients. The method can be easily programmed and its exactness is often considerably high.

An essential limitation of this approach is that a fundamental solution of the corresponding partial differential operator should be explicitly known. This is generally not the case, if the original differential equation contain some coefficients that vary from location to location (e.g. electrical, thermal or hydraulic conductivity). Another problem arises when the equation is inhomogeneous, i.e. some source density terms appear in the right hand side.

In this talk, a localization technique is proposed, which converts the original problem to a sequence of subproblems defined on much smaller overlapping subdomains. In the local subdomains, the coefficients of the differential equation can be considered constant; thus, the MFS can be applied. The local subproblems are solved sequentially, in an iterative way. This mimics a multiplicative (alternating) Schwarz method. The localization technique makes it possible also to handle the appearing inhomogeneous terms. Due to its advantageous numerical properties, the technique can be considered a useful generalization of the MFS. The method is illustrated through numerical examples.

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AI-Driven Protein Design for Next-Generation Therapeutics

Ambrus Gordos, Attila Horváth, Gábor Oroszlán, Péterfi, Márton Megyeri

Many challenging pharmacological targets remain elusive to conventional therapeutics such as monoclonal antibodies (mAbs) and small molecules, largely due to limited accessibility and homologous "off-target" structures. Small molecules often lack the necessary selectivity while mAbs are hindered by steric limitations and the risk of unwanted immune responses.

Our innovative approach utilizes miniproteins—specialized, small-sized proteins that can strongly and specifically bind to drug targets without triggering undesirable immune responses. Furthermore, the compact size and rigid structure of miniproteins make them ideal candidates for computational design.

At VRGTx, we have developed the proprietary AI-MPRO platform to generate miniproteins with precision targeting. Our process begins with computational design, creating miniprotein scaffolds de novo for virtually any target. Our advanced AI stack incorporates diffusion models and neural networks tailored for protein design, leveraging data from both wet lab and computational experiments. With the computational power of Komondor HPC, our processes run in a fast-paced and iterative manner, making us competitive in the pharmaceutical industry. The computationally designed scaffolds are then refined through wet lab-based experiments using a unique, proprietary screening method that includes repetitive next-generation sequencing and big data analytics.

Our structure-function insights from sequencing data feed back into the AI stack, resulting in an iterative design-build-test-learn cycle that integrates wet lab and computational efforts. This approach shortens development timelines, reduces costs, and significantly enhances the quality of potential therapeutic candidates, resulting in safer and more effective therapeutics.

Ambrus Gordos - VRG Therapeutics, Attila Horváth - The University of Melbourne; Gábor Oroszlán - VRG Therapeutics, Péterfi Zalán - VRG Therapeutics, Márton Megyeri - VRG Therpautics

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Sound Speed and Layer Adapted Focusing Methods in Medical Ultrasound

Simon Hackl, Prof. Ronny Ramlau, Simon Hubmer

Focused ultrasound is a widely used non-invasive diagnostic and therapeutic tool in modern medicine. A crucial assumption in of its all applications is a constant sound speed in the observed medium. Non-constant sound speeds lead to actual times of flight of the ultrasound waves through the medium differing from calculated times of flight accounted for in focusing algorithms. This leads to an aberrated focus, which causes problems in applications. Although algorithms able to calculate the correct times of flight exist, they are too slow for the little computation time available in medical ultrasound imaging. Therefore, a significantly faster aberration correction method is needed. In this talk, we present adapted ultrasound focusing algorithms based on geometrical acoustics that make a step into this direction. In a known layered medium setting, it is possible to calculate the correct times of flight. The resulting adapted focusing algorithms correct for the aberrations caused by the different sound speeds in the medium layers. Existence and uniqueness conditions for a solution to the underlying system of equations are given. Furthermore, numerical simulations to determine the precision of our methods are conducted.

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A frequency domain solution for automotive transmission systems

Josef Haslinger, Klaus-Dieter Bauer, Günter Offner

This contribution deals with the solution of the equations of motion of a multibody system in frequency domain. When interested in steady-state operating conditions of automotive transmission systems under periodically varying external excitations, the simulation in time domain leads to very accurate results. However, transient oscillations from fast moving components may decay slowly. Frequency domain solutions (FDS) do not resolve this initial transient phase and can therefore reduce the computational effort substantially.

The multibody system representing the transmission system consists of rigid and/or flexible bodies based on FEM discretization. These bodies are interconnected by nonlinear elements (joints), which represent forces and moments from radial and axial bearings and from gear interactions.

Based on the linearized equations of motion along a reference trajectory, the FDS workflow is described in detail. In a first step, a kinetostatics solver is applied, where a loaded configuration of the model is sought for: external loads are applied and a static equilibrium position is computed leading to preloaded bodies and joints. In particular, gear contacts are being closed. At the preloaded equilibrium configuration, the system is linearized including joints, which are typically linearized by the method of finite differences. As a result, constant stiffness and damping coefficients are determined for each component of the system and assembled into mass, damping and stiffness matrices of the whole model. Next, external loads are transformed into frequency domain by using FFT. These external loads include gear contact excitations, which are considered through a "Tooth Contact Analysis", where periodic excitations induced by gear meshing effects are precomputed on a simplified model. Finally, for the dynamic solution in frequency domain, a linear equation system including mass, damping, and stiffness matrices of the system is solved for each loaded frequency component.

The FDS approach is validated on a simple gearbox model.

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Current and future challenges of mobility

Csongor Horváth

Nowadays, the field of mobility is facing greater challenges than ever. The different legislations worldwide are moving this sector towards the reduction of the CO2 emissions. This makes it necessary to research & develop vehicles with alternative powertrain systems that can fulfil the requirements of these legislations.

As far as the options are considered, the five most notable technologies are: the battery electric vehicles, the hybrid vehicles, the hydrogen fuel cell vehicles, the hydrogen fuel based internal combustion engine vehicles and the synthetic fuel based internal combustion engine vehicles. All of these technologies have their justification for existence and the best-suited applications are different for each one of them.

The aim of this presentation is to give a short introduction into these technologies, outlining their advantages & drawbacks from the different perspectives and to select the best applications for each of the alternative powertrain vehicles.

Besides this purpose, the presentation will focus on the currently emerging technologies in the field of electric drive systems, which are expected to transform this field and also present interesting research & development challenges for the future.

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Efficient room acoustic simulations

Ferenc Izsák

A room acoustic simulation is introduced based on the recent techniques. A frequency-dependent model of reflections is used. In the corresponding equations, this results multiple boundary delays. The spatial discretization is performed using a recent family of mass lumping finite elements. For the time discretization, a second a third order extension of a recent symplectic method was developed. The numerical method is tested on a real-life situation by simulating the sound propagation in a car interior.

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Using Functional Mock-Up Units for Multi-Physical System Simulation in Electric Vehicle Development

Michael Kolmbauer, Björn Liljegren-Sailer, Günter Offner, Ralf Uwe Pfau

Today, physical prototypes are being replaced by digital twins wherever possible. The key factors are the high quality of the digital twins and the increasing usability of the corresponding software. Due to current trends such as electrification and heterogeneous drive concepts, the number of subsystems in a vehicle is increasing, which leads to more complexity in the overall system. The challenges in developing future vehicles lie not only in the design of the powertrain as a single component, but also in the assessment of the entire vehicle, including passenger comfort. This requires interdisciplinary knowledge on the one hand, but also a clear strategy that enables a working framework across disciplines.

In this talk, we show dedicated use cases from multi-physical system simulation where specialized mathematical frameworks can be used to achieve these goals. The focus is not only on the development of powerful simulation tools for the individual components, but also on the stable interaction within multi-physical systems. This becomes even more challenging when parts of the multi-physical system are replaced by black-box models representing controllers, individual components, or even complete circuits. For automotive applications, the Functional Mock-up Interface (FMI) has been established as a standard for black box models that defines a container (FMU) and an interface (FMI) for exchanging dynamic simulation models. The integration of FMUs in multi-physical system simulation can be done on different levels (model exchange, co-simulation) and can lead to solvability, index and stability issues that need to be addressed.

Michael Kolmbauer – MathConsult GmbH, Björn Liljegren-Sailer - Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austrian Academy of Sciences, Günter Offner, Ralf Uwe Pfau - AVL List GmbH

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Interpretable representation learning by means of variable projections

Péter Kovács

Although deep learning (DL) models have made significant strides in various domains in recent years, they often have strong data dependence, are prone to provide inconsistent predictions on unseen data, and fail to learn explainable relationships between input and output variables. These limitations of purely data-driven models are crucial in many applications, such as healthcare, automatization, and control, which requires reasonable and trustworthy decision making. Addressing these issues is essential to accomplish commercial standardization of artificial intelligence technologies.

The previously mentioned shortcomings are mainly due to the model-agnostic learning approach which relies purely on data and discards domain knowledge. Therefore, we propose VPNet, a novel model-driven DL architecture by combining variable projections (VPs) and neural networks. VP is a classical method for solving separable nonlinear least squares problems (SNLLSs) by which we extract features automatically in our learning framework. Note that many inverse problems can be formulated as SNLLS data fitting problems including a small set of adjustable nonlinear parameters with direct physical interpretations. Therefore, VPNet retains the powerful learning ability of DL methods, and the representation abilities of VPs in which both the trainable parameters and the extracted features are interpretable. In this talk, we present the VPNet concept and demonstrate its effectiveness in three real-world applications: DC motor identification, smart tire development, and EEG signal classification.

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Torque calculation methods for synchronous reluctance machines of eMobility

Richárd Csaba Kovács, Vilmos Paiss

Electric powertrain systems are getting more and more popular today. Currently the most frequently used traction machine type is the permanent magnet synchronous motor (PMSM) as in general it has a high efficiency and high power/torque density. However, these advantages are compromised by the numerous disadvantages of the machine. Most of these disadvantages are caused by the permanent magnets themselves.

A potential solution to achieve high efficiency and at the same time eliminate the need for the permanent magnets could be the application of the synchronous reluctance motors (SynRMs). These are also synchronous machines with high efficiency, and they do not utilize permanent magnets for the torque production. However, SynRMs have a much more nonlinear behavior than PMSMs. The stator inductances are changing with the rotor position and the stator currents, too. This requires advanced methods for the modelling of the machine including the computation of the electromagnetic torque.

The topic of this presentation is to introduce new torque calculation possibilities for SynRMs, that provide higher accuracy and also present excellent opportunities for the modeling of the machine.

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Space-time least-squares FEM for convection-diffusion problems

Christian Köthe, Olaf Steinbach

Instationary convection-diffusion problems arise in many applications, such as e.g., pollution simulations, heat transfer problems between thin domains, or in the modelling of flow and transport problems, to name but a few. In the advection-dominated case, the solutions are characterised by boundary layers, which lead to numerical instabilities and hence unphysical solutions when discretised with standard finite element methods. Known strategies to obtain stable solutions include the Streamline-Upwind Petrov-Galerkin (SUPG) method or a residual minimisation/least-squares approach. In this talk we focus on the latter approach. We will present an abstract least-squares framework that includes a built-in error estimator that can be used in a space-time adaptive refinement scheme. Furthermore, we will show that the instationary convection-diffusion equation fits into this framework and conclude with numerical examples that confirm our theoretical findings.

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Elektro-Thermal Topology Optimization of an Electric Machine

Nepomuk Krenn, Peter Gangl

We consider the multi material design optimization problem of a permanent magnet synchrounous machine in magnetostatic operation where we aim to maximize the average torque for a fixed amount of permanent magnets. Assuming a sufficiently good cooling of the stator we are interested in controling the heat in the rotor produced by the eddy currents in the permanent magnets in order to avoid demagnetization caused by temperature. For this we use the eddy currents of a whole electric period as the source term of a linear heat equation. As a first approach we solve the design optimization problem considering the electro-thermal coupled system imposing a pointwise temperature constraint. The resulting design comes with a reduction of the torque while respecting the temperature constraint. In the second approach we first optimize the magnetic properties only and add in a second step heat pipes which realize a passive cooling in order to conduct the heat out of the machine. We optimize the topology of the heat pipes neglecting their magnetic effects.

The design is represented by a level set function and updated by the topological derivative, a pointwise sensitivity of the cost functional subject to material changes. We derive the topological derivative of the coupled system using an adjoint method and present optimization results.

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ProkBERT: genomic language models for understanding the microbiome

Balázs Ligeti, Judit Juhász, Dániel Krizsán, János Juhász, Babett Bodnár

Investigating the microbiome's complexity requires advanced analytical tools capable of interpreting complicated and sparse datasets. Common problems like different types of data and low signal-to-noise ratios make it hard to use traditional machine learning methods effectively in microbiome research. Our research introduces a family of transformer-based neural networks to generate robust, generalizable sequence representations tailored to microbes, which helps to overcome specific challenges in microbiome analysis

By using the benefits of transfer learning, ProkBERT family is designed to analyze the detailed, yet complex, datasets inherent in microbiome research. Different from standard models, it uses a self-supervised learning approach, which helps understand unlabeled genetic sequences better. Our new Local Context-Aware (LCA) tokenization method goes beyond usual tokenization by keeping a closer look at the local sequence details, making the model's predictions more accurate. Comparative studies demonstrate that ProkBERT not only retains a richer local context but also adjusts more easily to various bioinformatics tasks, outperforming existing models in terms of precision and adaptability.

We’ve applied these models to specific challenges, including phage identification, lifestyle prediction, and determining phage-host relationships. While tackling promoter identification, ProkBERT reached an MCC of 0.74 for E. coli, demonstrating its utility in precise scenarios. Additionally, in broader tasks like phage sequence identification, our model outperformed competitors like VirSorter2 and DeepVirFinder with an MCC of 0.85, proving its broad applicability and ease of use.

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Structure-preserving model reduction of network systems

Bjoern Liljegren-Sailer

Many modern applications in the applied sciences require the simulation, control, and optimization of very large dynamical systems. One way to deal with the resulting high computational cost and time is to approximate such large-scale dynamical systems with reduced models obtained by model order reduction methods. Specifically, the snapshot-based methods have been successfully used in numerous applications. However, it has also been observed that the standard model reduction methods can suffer from poor stability issues and related performance degradation. Due to the latter, structure-preserving model reduction methods have recently gained attention. By preserving or mimicking relevant geometric structures such as, e.g., conservation laws or symplecticities, unphysical solution behavior and numerical instabilities can be avoided in many cases.

In this talk, we will give a brief overview of the model order reduction approach and discuss the issue of structure-preservation using coupled flow problem on networks as an example. The structure-preserving part will be based on energy-based modeling concepts, specifically the port-Hamiltonian approach.

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Air flow simulation of large scale forced draught cooling cells for power plant

Máté Márton Lohász

MVM EGI is traditional player on the dry cooling market for power plants. One important technique for the dry cooling is to use Air Cooled Condensers (ACC). The most established type of ACC is the forced mechanical draught arrangement where the cooling air is forced by an axial fan through the heat exchanger bundles. In this configuration the bundles are placed in an A shape above the fan. For power plant applications many (even one hundred) such ACC cooling cells needs to be arranged in a matrix. The various meteorological conditions (mainly the wind) are affecting the performance of the cooling system. Since the actual effect remarkably influenced by both the actual cooling system design and the surrounding buildings computational fluid dynamics (CFD) simulation is required to quantify and/or mitigate these effects. Since such cooling systems are huge, simplifications and optimisation of the computational procedure is (even in position of supercomputers) is a must. In the presented approach both the fans and heat exchangers bundles are modelled in a self-developed porous zone computationally efficient approach. The meshing strategy is also tuned for this purpose as will explained in the proposed presentation.

These simulation results in the proposed optimised way can be used also in design phase to find optimal fan selection and geometry arrangements to find the required balance of investment and operational cost.

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Thermal Analysis of Hydrodynamic Lubricated Journal Bearings in Automotive and Industrial applications

Norbert Lorenz, Günter Offner

Hydrodynamic journal bearings are central components in combustion engines, in gearboxes such as those found in wind turbines, and in aircraft turbofans. Predicting their reliability, service life and cost-effectiveness, as well as reducing frictional power losses and wear, are key issues in simulating oil-film-lubricated bearing contacts in such engines.

In this work, a thermo-elasto-hydrodynamic contact model is presented, which computes the temperature distribution within the thin viscous lubrication film and the temperature in the neighbouring bearing shell and journal structures. The oil film temperature is solved by using the energy equation. The equation contains convection and conduction terms, a thin film approximation for the dissipation term, the effect of thermal expansion and transient effects. Besides component material properties such as specific heat capacity, density, heat conductivity for lubricant and structures, also heat transfer through mixed lubricated regimes and partly filled clearance gaps, as implied in cavitation regions, are being considered. The equation also includes surface roughness of the contacting journal and shell structures. In the areas of oil supply, a mixing process takes place, where cold supply oil mixes with hot re-circulated oil within the journal bearing clearance. The bearing shell and journal structure temperatures are based on the three-dimensional thermal conduction equation with material dependent conductivity and contain the heat source due to dry asperity contact. Boundary conditions are described for these equations followed by material properties and the local flow conditions in the fluid.

These thermal processes are known to be inert compared to structural dynamics. Long simulation times to cover transient thermal behaviour and to reach the operating temperature of the system may be the consequence. In order to reduce the simulation time in such cases, a heat-up acceleration algorithm is applied.

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Modelling synchronization phenomena in brain and power-grid networks

Géza Ódor, István Papp, Bálint Hartmann, Kristóf Benedek

Synchronization phenomena are very abundant in nature. Brain signals are the most obvious occurrences measured by EEG. Too much synchronization is not welcomed, as it leads to seizures. There is a hypothesis, strengthened by many experiments and models, that brain operates slightly below or at the critical point. That is also optimal for information processing, not only in natural, but in artificial networks, like reservoir computers. Synchronization is very much the target in case of power-grids, however socio-techno-economic factors organize such systems close to criticality, dictated by the finite resources of supply and demand. Most fundamental models of both applications are Kuramoto type differential equations, which we solve using GPU accelerated HPC CUDA algorithms.To see critical scale-free behavior we need to consider large networks that require very strong computational resources. Recently we have shown that criticality also has positive consequences for power-grids. Braess paradox and islanding desynchronization can be avoided.

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A novel motor model for synchronous reluctance machines of electric vehicles

Vilmos Paiss

Electric vehicles are getting more and more focus today due to the different legislations related to the CO_2 emissions. Although, the currently most frequently used Permanent Magnet Synchronous Machines (PMSM) offer excellent efficiency in numerous operation zones, they suffer from serious drawbacks and most of them are caused by the rare earth permanent magnets.

This makes it necessary to develop alternative motor solutions that also offer excellent efficiency and at the same time do not utilize rare earth permanent magnets. One of the promising alternatives are the synchronous reluctance motors. These are also synchronous machines, which is one of the reasons why they have excellent efficiency. However, they present a heavily nonlinear behavior mainly due to the varying stator inductances that are a function of many different input variables. Therefore, new modeling methods are required to give a more accurate representation of the machine behavior.

The topic of this presentation is to introduce a new motor modeling method for synchronous reluctance machines, which can give a more precise description of the machine and can be utilized well by the system designing- and the motor control algorithm development activities.

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Computational methods for cardiac catheter ablation procedures

Argyrios Petras, Luca Gerardo-Giorda

Catheter ablation is a common treatment for severe cardiac arrhythmias. During the procedure, a catheter is typically inserted through the patient's groin and guided into the cardiac chamber, where it inflicts targeted damage to arrhythmogenic tissue in order to restore normal sinus rhythm. Two primary ablation technologies are used: thermal-based techniques like radiofrequency ablation (RFA) and non-thermal approaches such as pulsed field ablation (PFA), which uses pulsed electric fields to induce cellular electroporation. While these methods are generally safe and effective, further research is required to improve lesion durability and reduce procedural complications.

In this presentation, we introduce our computational models for simulating these two dominant ablation techniques, RFA and PFA. Leveraging a multiphysics approach and account for the multiscale phenomena involved, from the cellular level to the tissue and organ scale, we develop digital twins that accurately capture the lesion formation process. We present the applications to different aspects of the procedure, and also our strategies for extending these models to support personalized medicine and in-silico clinical trials.

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Parametric Optimization of Electric Machines

Siegfried Silber

The design of electrical machines requires the integration of several interdependent physical domains, including electromagnetic, thermal, structural, and acoustic analyses. Optimizing performance in one domain often adversely affects another; for example, achieving superior electromagnetic properties may negatively affect the mechanical strength of the rotor. This paper presents a comprehensive approach to parametric optimization that simultaneously considers these conflicting requirements. The use of genetic optimization algorithms is explored to effectively navigate the complex multidimensional design space. In addition, accelerated optimization techniques using surrogate models are introduced to reduce the computational burden while maintaining accuracy. The proposed methodology aims to improve the overall performance and reliability of electrical machines by balancing the trade-offs between competing physical constraints.

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Innovation and competitive advantage: The new paradigm for the collaboration between the academy and the industry

István Szászi

The history of the technological advancements has been regularly witnessing paradigm shifts which are accompanied by major technological leaps. Generally, in these situations the former market leaders have become comfortably accustomed to the incremental development approach, improving only a small portion of the state-of-the-art solution. On the contrary, the edible players have been quick to recognize the changing market demands and have come up with novel, innovative solutions that can satisfy them, thereby gaining market leadership.

The incremental improvements – which are one of the key strengths of the industry – play an important role in maintaining the market leadership position on short- and medium terms. However, it is essential to keep a constant eye on the market needs and to regularly reevaluate the technology from its fundamentals. The latter is a key strength of the academia.

Today, we are on the verge of a paradigm shift in the field of electric vehicle drive systems. The currently widely used permanent magnet synchronous motor based propulsion systems are essentially incrementally developed solutions adopted from the industry. This creates several problems that prevent the wider uptake of the electric vehicles and their acceptance by the users. This makes it necessary to abandon the incremental development approach and to create fundamentally new and innovative drive solutions.

The researchers of the Robert Bosch Kft. have developed an axial-flux synchronous reluctance motor based drive system that offers a solution to the problems of the current drives and is a prime example for the synergic combination of the academic- and the industrial ways of thinking. Our researchers have been working closely with the academia from the beginning, uniting the strengths of both spheres. The cooperation has further enormous potential, and its exploitation should be a role model for the new joint industry-academia collaboration.

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Reluctance motor drives: an opportunity to a more sustainable electric transportation

Tibor Vajsz

The field of the electric vehicle propulsion systems is struggling to find highly efficient and competitive drive system solutions. Although the currently most widespread permanent magnet synchronous motor (PMSM) drives in general offer excellent efficiency and high power-density but they are affected by serious drawbacks. Most of these drawbacks are originated from the permanent magnets themselves, which due to several reasons use rare-earth elements as base materials.

These rare-earth base materials are costly and suffer from serious geopolitical issues because China dominates their supply chain. This leads to unstable base material prices which poses high risks to the economical turnout of a development project. All these problems make the PMSM drives a less competitive choice for traction systems of electric vehicles.

Besides the economical aspects, the rare-earth materials have other disadvantages. For example, their mining is highly polluting. In addition, the permanent magnets make the PMSMs sensitive to overcurrent, overheating and vibration. An additional derating has to be applied for the machine to prevent the demagnetization of the permanent magnets on the rotor.

A potential solution for these problems could be the application of the reluctance motors. These are also synchronous-type motors, thus offering excellent efficiency. Unlike the PMSMs, they do not need any permanent magnets for the torque production.

The aim of this presentation is to give an introduction to the field of the reluctance motor drive systems and to present their most important characteristics. The research & development challenges that are related to the designing- and the controlling of these drive systems will be shown as well.

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Optimizing data fitting in ultrasound simulations: Exploring linear and nonlinear models

Huidong Yang, Peter Elbau, Michael Figl, Otmar Scherzer, Lukas Zalka

We present our work on optimizing the fitting process between experimental ultrasound data and forward modeling of ultrasound propagation in water. Our approach employs numerical approximations of both linear and nonlinear physical models for simulations, with experimental data provided by our collaborators at the Medical University of Vienna. We emphasize the subtle differences in how the linear and nonlinear models fit the experimental data.

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