ECMI 2023

22nd ECMI Conference on Industrial and Applied Mathematics

June 26 – 30, 2023
Wrocław, Poland

Contents

Part I

Introduction

The European Consortium for Mathematics in Industry (ECMI) conferences aim to enforce the interaction between the academy and industry, leading to innovations in both fields. These events have attracted leading experts from business, science and academia, and have promoted the application of novel mathematical technologies to industry. We hope that ECMI 2023 will further enhance multidisciplinary research and development both in academia and industry, leading to the formulation of challenging real-life problems, where mathematics may provide significant new insights and, at the same time, may be inspired by those interactions.

The conference in Wrocław will be attended by about 300 people (including a group of 50 students), mainly from outside Poland. It consists of 26 minisymposia and 58 contributed talks. On Thursday, 29 June, we are planning the Industry Day, during which industry representatives will talk about how they apply modern mathematical tools in their companies. The speakers come from KGHM (Polish company, a major copper and silver producer in the world, also the main sponsor of the conference), BNY Mellon, Nokia, Santander, Satrev, Saule Technologies and Sun Cable, At the end of this day we organise an expert panel discussion on the future of industrial and applied mathematics moderated by Dirk Hartmann (Siemens).

Major application areas covered
Applied physics
Biology and medicine
Ecology
Cybersecurity
Climate
Data science
Economy, finance and insurance
Energy
Production systems
Social challenges
Transportation challenges

Selected topics covered
Cooperative games
Differential equations
Financial mathematics
Fluid dynamics
Information theory and statistics
Inverse problems
Machine learning
Network analysis
Risk processes
Signal processing
Topological data analysis

The social programme consists of the ECMI Welcome Reception on Monday evening where ECMI nodes will present their achievements in the form of posters (H-14 Building), Wrocław sightseeing with a guide on Wednesday afternoon (starting from the conference venue) and Gala dinner with concert on Thursday evening (Wrocław Congress Center, Centennial Hall complex).

Official patron of the conference
Prof. Arkadiusz Wójs, Rector of Wrocław University of Science and Technology

Plenary speakers and committees

Plenary speakers

- Ruth Baker, University of Oxford, United Kingdom
- Dirk Hartmann, Siemens, Germany
- Uwe Iben, Bosch, Germany
- Ron S. Kenett, Samuel Neaman Institute, Technion, Israel
- Irena Lasiecka, University of Memphis, USA
- Henrik Madsen, Technical University of Denmark, Denmark
- Mathilde Mougeot, École Normale Supérieure Paris-Saclay, France
- Claudia Schillings, Freie Universität Berlin, Germany
- Rafał Weron, Wrocław University of Science and Technology, Poland

Scientific Committee

- Krzysztof Burnecki, Wroclaw University of Science and Technology, Poland
- Ana Carpio, Complutense University of Madrid, Spain
- Matthias Ehrhardt, Bergische Universität Wuppertal, Germany
- Poul Georg Hjorth, Technical University of Denmark, Denmark
- Matylda Jabłońska-Sabuka, LUT University, Finland
- Nataša Krejić, University of Novi Sad, Serbia
- Alessandra Micheletti, Universita' degli Studi di Milano, Italy
- Jacek Miękisz, University of Warsaw, Poland
- Sarah Mitchell, University of Limerick, Ireland
- Jörg Osterrieder, University of Twente, Netherlands
- Jean-Michel Poggi, Université Paris-Saclay, France
- Peregrina Quintela, University of Santiago de Compostela, Spain
- Wil Schilders, Eindhoven University of Technology, The Netherlands
- Carola-Bibiane Schönlieb, University of Cambridge, UK

Local Organizing Committee

- Krzysztof Burnecki (Chair)
- Janusz Szwabiński (Vice-Chair)
- Marek Teuerle (Vice-Chair)
- Michał Balcerek
- Aleksandra Grzesiek
- Joanna Janczura
- Łukasz Płociniczak
- Jakub Ślęzak
- Mateusz Świtała
- Agnieszka Wyłomańska
- Monika Kaczmarz
- Anna Smyk
- Ewa Syta

Part II

General information

Registration Registration desk is located at the conference venue (Wrocław University of Science and Technology Congress Centre). Registration is available on Monday between 07:45 - 17:00 and on each other conference day between 8:30 - 15:00.

Conference Fees Conference fees cover: conference attendance, information material, lunches, coffee breaks and social events.

Coffee Breaks Coffee breaks are served at the conference venue.

Lunches Lunches are served in the buffet style at the conference venue. Lunch will be available only with the conference badge.

Internet Access Wireless internet is available throughout `eduroam`.

Instructions for speakers Each lecture room is equipped with a PC, pointer, video projector. The PC is provided with the following software: MS Office and Adobe Reader. Please be aware that each oral presentation has a standard 20+5 minutes slot.

Please note that the 5 minutes are devoted to questions. Presentation upload is necessary to be done before the start of the session. You can also use your own laptop, but, in that case, please be aware that the time for your talk will be reduced due to the change of computers.

An assistant will be available to help speakers with technical issues. If you have video or any other special feature, please test the presentation with the technician well in advance of your session.

If you have any problem, please contact organizers (you will recognize them by yellow badges)!

Part III

Conference program

Program

Monday, June 26, 2022

	Monday					
8:30–9:00	Opening & Awards					
9:00-10:00	Dirk Hartmann					
10:00-10:40	Coffee break					
	CR 10 AC	CR 10 B	CR 10 D	CR 113	CR 114	CR 115
10:40-11:05	MS21	MS2	MS6	MS4	MS12	MS11
11:05-11:30	MS21	MS2	MS6	MS4	MS12	MS11
11:30-11:55	MS21	MS2	MS6		MS12	MS11
11:55-12:20	MS21	MS2	MS6		MS12	MS11
12:20-13:50	Lunch					
13:50-14:50	Ron S. Kenett					
14:50-15:30	Coffee break					
15:30-15:55	MS21	MS2	MS17	MS8	MS12	CT2
15:55-16:20	MS21	MS2	MS17	MS8	MS12	CT2
16:20-16:45	MS21	MS2	MS17	MS8	MS12	CT2
16:45-17:10	MS21	MS2	MS17	MS8	MS12	CT2
17:10-17:20	Short break					
17:20-17:45	MS21	CT3	CT4	CT1	MS12	
17:45-18:10	MS21	CT3	CT4	CT1	MS12	
18:10-18:35	MS21	CT3	CT4		MS12	
18:35-19:00		CT3	CT4			
19:15	ECMI Welcome Reception					

Tuesday, June 27, 2022

	Tuesday					
9:00-10:00	Ruth Baker					
	CR 10 AC	CR 10 B	CR 10 D	CR 113	CR 114	CR 115
10:40-11:05	MS1	MS21	MS9	MS7	MS2	MS10
11:05-11:30	MS1	MS21	MS9	MS7	MS2	MS10
11:30-11:55	MS1	MS21	MS9	MS7	MS2	MS10
11:55-12:20	MS1	MS21	MS9	MS7		MS10
12:20-13:50	Lunch					
13:50-14:50	Henrik Madsen					
14:50-15:30	Coffee break					
15:30-15:55	MS1	MS21	MS9	MS7	CT5	MS10
15:55-16:20	MS1	MS21	MS9	MS7	CT5	MS10
16:20-16:45	MS1	MS21	MS9	MS7	CT5	MS10
16:45-17:10	MS1		MS9	MS7	CT5	MS10
17:10-17:20	Short break					
17:20-17:45	MS1	MS21	MS13	MS26	CT7	CT18
17:45-18:10	MS1	MS21	MS13	MS26	CT7	CT18
18:10-18:35	MS1		MS13	MS26	CT7	CT18
18:35-19:00			MS13	MS26	CT7	CT18

Wednesday, June 28, 2022

	Wednesday						
9:00-10:00	Claudia Schillings						
10:00-10:40	Coffee break						
	CR 10 AC	CR 10 B	CR 10 D	CR 113	CR 114	CR 115	CR 106
10:40-11:05	Anile Prize	MS23	MS14	CT8	MS18	MS19	CT9
11:05-11:30	Wacker Prize	MS23	MS14	CT8	MS18	MS19	CT9
11:30-11:55	MS25	MS23	MS14	CT8	MS18	MS19	CT9
11:55-12:20	MS25	MS23	MS14	CT8	MS18	MS19	CT9
12:20-13:50	Lunch						
13:50-14:50	Rafał Weron						
14:50-15:30	Coffee break						
15:30-15:55	MS25	MS23	MS14	CT6	MS18	MS20	CT11
15:55-16:20	MS25	MS23	MS14	CT6	MS18	MS20	CT11
16:20-16:45	MS25	MS23	MS14	CT6	MS18	MS20	CT11
16:45-17:10	MS25		MS14	CT6		MS20	CT11
17:10-19:00	Sightseeing						

Thursday, June 29, 2022

	Thursday	
9:00-10:00	Uwe Iben	
10:00-10:40	Coffee break	
	CR 10 AC	CR 113
10:40-12:20	KGHM, BNY Mellon × 2, Santander	MS5
11:05-11:30		MS5
11:30-11:55		MS5
11:55-12:20		MS5
12:20-13:30	Lunch	
13:30-13:55	Nokia, Sun Cable, Saule Technologies, SatRev	MS14
13:55-14:20		MS14
14:20-14:45		MS14
14:45-15:10		MS14
17:10-17:20	Short break	
15:20-15:45	MS22	
15:45-16:10	MS22	
16:10-16:35	MS22	
16:35-17:00	MS22	
17:00-17:10	Short break	
17:10-18:10	Panel Discussion: The Future of Industrial and Applied Mathematics	
19:00	Conference Gala Dinner	

Friday, June 30, 2022

	Friday						
9:00-10:00	Mathilde Mougeot						
10:00-10:40	Coffee break						
	CR 10 AC	CR 10 B	CR 10 D	CR 113	CR 114	CR 115	CR 106
10:40-11:05	MS16	MS14	MS15	MS24	MS25	MS3	CT16
11:05-11:30	MS16	MS14	MS15	MS24	MS25	MS3	CT16
11:30-11:55	MS16		MS15	MS24	MS25	MS3	CT16
11:55-12:20	MS16		MS15		MS25	MS3	CT16
12:20-13:50	Lunch						
13:50-14:50	Irena Lasiecka						
14:50-15:30	Coffee break						
15:30-15:55	MS16	CT17	CT15	CT12	CT14	MS3	
15:55-16:20	MS16	CT17	CT15	CT12	CT14	MS3	
16:20-16:45		CT17	CT15	CT12	CT14	MS3	
16:45-17:10		CT17					
17:10-17:40	ERC						
17:40-18:30	Closing Ceremony						

Part IV

Plenary lectures

QUANTITATIVE COMPARISONS BETWEEN MODELS AND DATA TO PROVIDE NEW INSIGHTS IN CELL AND DEVELOPMENTAL BIOLOGY

Ruth Baker

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Abstract: Simple mathematical models have had remarkable successes in biology, framing how we understand a host of mechanisms and processes. However, with the advent of a host of new experimental technologies, the last ten years has seen an explosion in the amount and types of quantitative data now being generated. This sets a new challenge for the field - to develop, calibrate and analyse new models to interpret these data. In this talk I will use examples relating to cell motility and proliferation to showcase how quantitative comparisons between models and data can help tease apart subtle details of biological mechanisms.

Bio: Ruth Baker is Professor of Applied Mathematics at the Mathematical Institute, University of Oxford. Her research sits at the interface of applied mathematics and the biomedical sciences. In particular, it focusses on the development and application of technologies to transform understanding of how cell-level biomechanical and biochemical mechanisms drive morphogenesis at the cell and tissue level. The tools she develops to analyse models draw upon ideas from a diverse range of subfields of mathematics and, importantly, theoretical developments are always motivated by, and embedded within the study of particular biological systems.

EXECUTABLE DIGITAL TWINS - INTEGRATING THE DIGITAL AND REAL WORLD

Dirk Hartmann

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Abstract: We live in a world of exploding complexity with enormous challenges. Digital twins, tightly integrating the real and the digital world, are a key enabler for decision making in the context of complex systems. While the digital twin has become an intrinsic part of the product creation process, its true power lies in the connectivity of the digital representation with its physical counterpart. To be able to use a digital twin scalable in this context, the concept of an executable digital twin has been proposed. An executable digital twin is a stand-alone and self-contained executable model for a specific set of behaviors in a specific context. It can be leveraged by anyone at any point in lifecycle. To achieve this, a broad toolset of mathematical technologies is required - ranging from model order reduction, calibration to hybrid physics- and data-based models. In this presentation, we review the concept of executable digital twins, address mathematical key building blocks such as model order reduction, real-time models, state estimation, and co-simulation and detail its power along a few selected use cases.

Bio: Dirk Hartmann is an industrial mathematician, Siemens Technical Fellow, intrapreneur, and thought leader in the field of Simulation and Digital Twin. Multiple of his innovations have led to novel products and services and have been showcased at top-level innovation events. Among many distinctions, he received the prestigious Werner-von-Siemens Top Innovator award 2019 for his life-time achievements and the Siemens Inventor of the Year 2021 award.

TAYLOR MAPPING AND POLYNOMIAL NEURAL NETWORKS FOR SOLVING FORWARD AND INVERSE ORDINARY DIFFERENTIAL EQUATIONS

Uwe Iben

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Abstract: Companies have a continuous need to drive their business forward by developing new products or by automating production process. Digital Twins refer to virtual simulation models of components or products which can imitate the use and properties in real time. The models also authentically simulate the product's natural user environment and its handling. Therefore, the development of technical components by digital methods and equipping the components with additional functions is becoming increasingly important. Many of the models are based on ordinary differential equations (ODEs) and most of the technical problems are inverse problems that are difficult to solve. One the one hand, they often contain parameters that are only partly unknown, e.g., material parameters. On the other hand, there are often only small amount of data available that can be used to solve the inverse problem. To overcome these challenges, novel methods are needed. In Taylor mapping (TM), the solution of the ODE with respect to the initial values is developed into a polynomial series. The associated Taylor weights are computed using ODEs and are valid for each initial value problem of this ODE. The approach of TM can be used for the calculation of the solution of the inverse problem. The underlying ODE has not to be known explicitly. The Taylor weights are computed by solving a least square problem with respect to the discrete time values of the time series. This algorithm can be interpreted as a Polynomial Neural Network (PNN) where the neurons are polynomials, and the layers present a certain polynomial order. The Taylor Mapping and PNN approach is demonstrated and analyzed on academic examples. The accuracy and the forecast of the solution are in focus. Further, a catalytic reaction is presented as a realworld application.

Bio: Uwe Iben is an engineer and applied mathematician at Central Research and Advance Engineering of Robert Bosch GmbH. He worked for more than 15 years as a chief expert on the field of cavitation and multi-phase flow and developed models and numerical schemes for simulation of cavitation and cavitation induced erosion. He is currently working as a chief expert on methods for solving differential equations using AI methods. Since 2017, he has been an honor professor at the University of Stuttgart.

ENGINEERING, BIG DATA, AND THE FUTURE

Ron S. Kenett

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Abstract: Advancements in technology and data access are followed by significant changes in the scope of engineering work. In Industry 4.0 sensor technologies enable improved monitoring, diagnostic, prognostic and prescriptive analytic capabilities providing systems and processes with a digital asset that parallels the physical assets. This evolution triggers a shift from engineering of design to engineering of performance. This change involves an integration of mathematical models, driven by physics, with statistical and analytic data driven models. In this context, differential and partial differential equations are combined with empirical models to provide enhanced precision and generalizability. Topics of current interest include hybrid models, soft sensors, digital twins and model order reduction methods. The talk will review this background and sketch future pathways emphasizing engineering of performance, in contrast to engineering of design. This conceptual shift repositions the role of model-based system engineering (MBSE) and detailed requirement analysis as systems are increasingly considered "porous" with upfront incomplete requirements. Particular attention will be given to systems of systems that are extremely large, extremely uncertain and extremely complex. The talk makes the case that the goal of engineering for performance is to achieve optimal decision-making with high accuracy in almost real-time. A case study from the Israeli railway system will be presented.

Bio: Professor Ron Kenett is Senior Research Fellow at the Samuel Neaman Institute, Technion, Haifa, Israel Chairman of the KPA Group, Israel, Chairman of the Data Science Society at AEAI and Research Professor at the University of Turin, Italy. He is an applied statistician combining expertise in academic, consulting and business domains. Ron is member of the Public Advisory Council for Statistics Israel, member of the of Digital Twin Center of Excellence (DiTCE) at Ben Gurion University of the Negev, member of the INFORMS QSR advisory board and member of the advisory board of DSRC, the University of Haifa Data Science Research Center. He is Past President of the Israel Statistical Association (ISA) and of the European Network for Business and Industrial Statistics (ENBIS). He authored/co-authored over 250 papers, 18 books on data science, industrial statistics, biostatistics, healthcare, customer surveys, quality control, risk management, software testing, and information quality. The KPA Group, he founded in 1994, is a leading Israeli firm focused on generating insights through analytics. He was awarded the 2013 Greenfield Medal by the Royal Statistical Society, in 2018, the George Box Medal by the European Network for Business and Industrial Statistics and, in 2022, the life achievement award by the Israeli Society for Quality. He earned a BSc in Mathematics (with first class honors) from Imperial College, London University and a PhD in Mathematics from the Weizmann Institute of Science, Rehovot, Israel.

CAN WE CONTROL A FLUTTER IN FLOW-STRUCTURE INTERACTIONS?

Irena Lasiecka

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Abstract: Flow-structure interactions are ubiquitous in nature. Problems such as attenuation of turbulence or flutter in an oscillating structure [Tacoma bridge], flutter in tall buildings, fluid flows in flexible pipes, in nuclear engineering flows about fuel elements and heat exchanger vanes - are prime examples of relevant applications. Mathematically, the models are represented by a 3D compressible, irrotational Euler Equation coupled to a nonlinear dynamic elasticity on a 2D manifold. Strong boundary-type coupling at the interface between the two media is at the center of the analysis. This provides for a rich mathematical structure, opening the door to several unresolved problems in the area of nonlinear PDE' s, dynamical systems, related harmonic analysis and differential geometry. This talk aims at providing a brief overview of recent developments in the area along with a presentation of some recent advances addressing the issues of control and long time behavior of such models.

Bio: Irena Lasiecka is the Distinguished University Professor at the University of Memphis and a former Commonwealth Professor at the University of Virginia. She received her PhD (1975) in Applied Mathematics from the University of Warsaw. She then spent 3 years at UCLA in a Post-Doc position, followed by Professorships at the University of Florida and the University of Virginia until 2013. She has also held numerous visiting appointments including Universite de Liege, the IMA at the University of Minnesota, the University of Bologna, UCLA, the Scuola Normale Superiore di Pisa, the University of Warsaw. Her research interests are in the general area of control theory for infinite dimensional systems - predominantly Partial Differential Equations (PDEs) with applications to interactive structures such as they arise in flutter control in aero-elasticity, turbulence suppression in fluids, noise attenuation in acoustic chambers, etc In this area she has published 5 research monographs and over 300 research papers. Her work was cited over 9,000 according to MathScinet and over 18,800 according to Google Scholar with H index = 68. Her work has been funded by NSF, AFOSR, ARO and also NASA. She has been in the ISI' s List of Highly Cited researchers since its inception. She was an IEEE Distinguished Lecturer, and a frequent Plenary Speaker at SIAM, AMS, IFIP, AIMS Conferences. She served as an associate editor of many journals including: IEEE Transactions on Automatic Control, Automatica, Systems and Control Letters, Siam Journal on Control, Journal of Optimization Theory and Applications, Applied Mathematics and Optimization, Journal of Mathematical Analysis and Applications, Nonlinear Analysis, Discrete

and Continuous Dynamical Systems. She is Editor-In-Chief [jointly with Roger Temam and Huyen Pham] of Applied Mathematics and Optimization [Springer] as well as of Evolution Equations and Control Theory [AIMS], jointly with Alain Haraux. She has been involved in leadership positions with IFIP [International Organization of Information Processes], including chair of the TC7-Committee on Modeling and Optimization. She has advised over 30 PhD students, several of whom have then pursued successful academic careers of their own and are now leaders in the field. She is a 2004 IEEE Fellow, 2019 SIAM Fellow and 2015 AMS Fellow. In 2011 she has was awarded the 2011 SIAM W.I. Reid Prize for contributions to control theory and differential equations. In 2019 she was awarded by AACC [American Automatic Control Council] the Richard Bellman Control Heritage Award for her contribution to boundary control of distributed parameter systems, 2020 William Sparks Eminent Faculty Award from Board of Trustees TN, and 2021 Hugo Steinhaus Award from Polish Mathematical Society. She was appointed Eisenbud Research Professor at MSRI, University of California, Berkelay for the semester on Mathematical Theory of Fluid Dynamics, 2021.

FORECASTING FOR THE WEATHER-DRIVEN ENERGY SYSTEM

Henrik Madsen

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Abstract: The transition to a future weather-driven and low carbon society implies that the energy system will undergo a fundamental change from a system where the production follows demand to a system where the demand follows the renewable power production. This also implies that access to state-of-the-art methods for forecasting will become important. In this talk recent developments in methods for renewable energy forecasting will be described. We will focus on methods for multivariate probabilistic forecasting of load, prices and renewable power generation. It will be argued that tools for integrated forecasting across domains (wind, solar, load, prices, ...) will become essential, and replace more silo-oriented tools for individual areas like wind power. It will be demonstrated that full multivariate probabilistic forecasts are important to obtain reliability and profitability in the operation of the future low-carbon energy system. Real-life decision problems often involve forecasts for multiple levels of a hierarchy. For instance it becomes essential that reliable and forecasts on all grid levels are coherent such that e.g., forecasts provided for wind farm owners, the DSO (distribution system operator) and the TSO (transmission system operator) are aligned. Reconciliation ensures unified forecasts that support aligned decisions across all levels of a hierarchy, whether it is cross–sectional, temporal, or spatial. This talk describes some of the recent developments in forecasting using both spatial and temporal hierarchies.

Bio: He got a PhD in Statistics at the Technical University of Denmark in 1986. He was appointed Ass. Prof. in Statistics in 1986, Assoc. Prof. in 1989, and Professor in Mathematical Statistics with a special focus on Stochastic Dynamical Systems in 1999. In 2017 he was appointed Professor II at NTNU in Trondheim. His main research interest is related to analysis and data-driven modelling of dynamical systems. This includes signal processing, time series analysis, model building, estimation, grey-box modelling, digital twins, prediction, optimization and control. The applications are mostly related to the digital transformation of the energy and water systems. He has got several awards. Lately, in June 2016, he was appointed Knight of the Order of Dannebrog by Her Majesty the Queen of Denmark, and he was appointed Doctor HC at Lund University in June 2017. He has authored or co-authored approximately 650 papers and 12 books. The most recent books are Time Series Analysis (2008); General and Generalized Linear Models (2011); Integrating Renewables in Electricity Markets (2013), and Statistics for Finance (2015).

MACHINE LEARNING DESIGN FOR INDUSTRIAL SMALL DATA REGIMES

Mathilde Mougeot

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Abstract: In recent years, considerable progress has been made in the implementation of decision support procedures based on machine learning methods through the exploitation of very large databases and the use of learning algorithms. In the industrial environment, the databases available in research and development or in production are rarely so voluminous and the question arises as to whether in this context it is reasonable to want to develop powerful tools based on artificial learning techniques. This talk presents research work around transfer learning and hybrid models that use knowledge from related application domains or physics to implement efficient models with an economy of data. Several achievements in industrial collaborations will be presented that successfully use these learning models to design machine learning for industrial small data regimes and to develop powerful decision support tools even in cases where the initial data volume is limited.

Bio: Mathilde Mougeot is Professeur of Data Science at Ecole Nationale Supérieure d'Informatique pour l'Industrie et l'Entreprise (ENSIIE) and adjunct Professor at ENS Paris Saclay where she holds the Industrial Research Chair "Industrial Data Analytics & Machine Learning". Since the beginning of her career, Mathilde Mougeot has been interested in machine learning for artificial intelligence applications. Her research activity is motivated by questions related to concrete applications stemming from collaborative projects with the socio-economic world. Her research focuses mainly on scientific issues related to predictive models in various contexts, such as those of high dimensionality, model aggregation, domain adaptation, data frugality by model transfer or by hybrid models. From 1999 to 2005, she has been contributed to the creation and the development of the start-up Miriad Technologies, specialized in the development of mathematical solutions for the industry based on machine learning, statistics and signal processing techniques. From 2016 to 2019, she was scientific officer for technology transfer in the Mathematics Division of Centre National de la Recherche Scientifique (CNRS) France. She offers a strong experience in leading projects at the interface of academics and industry.

PDE-CONSTRAINED OPTIMIZATION UNDER UNCERTAINTY

Claudia Schillings

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Abstract: 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.

Bio: Claudia is a Professor in Numerical analysis of stochastic and deterministic partial differential equations at Free University Berlin. Her research interests focus on the development of efficient methods for large-scale optimization problems in the presence of uncertainty in measurements, models, and parameters. Claudia received her PhD degree from the Department of Mathematics, University of Trier (Germany) in 2011. After two and half years of postdoctoral activity at ETH Zurich (Switzerland) and two years at the University of Warwick (UK), she was visiting professor at the Humboldt University Berlin (Germany) in 2015 - 2016 and then moved to Mannheim in 2017. In March 2022, she joined Free University Berlin. She has been working on a unified framework for the proper treatment of uncertainties in inverse and optimization problems for complex applications. Recent work includes the design of preconditioners for sampling techniques in the small noise or large data limit, data-informed approximations of the underlying model, and the analysis of particle-based methods for inverse problems.

RECENT ADVANCES IN ELECTRICITY PRICE FORECASTING: A 2023 PERSPECTIVE

Rafał Weron

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Abstract: Electricity price forecasting (EPF) is a branch of energy forecasting on the interface between econometrics/statistics, computer science and engineering, which focuses on predicting the spot and forward prices in wholesale electricity markets. Over the last 25 years, a variety of methods and ideas have been tried for EPF, with varying degrees of success. In this talk I will review recent developments in this fascinating area, including (but not limited to) probabilistic forecasting, combining forecasts and deep learning.

Bio: Rafał Weron is Professor of Management Science and Head of the Department of Operations Research and Business Intelligence at the Wrocław University of Science and Technology. He is one of the leading world experts on energy forecasting and is periodically engaged as a consultant to financial, energy and software engineering companies. Details on current projects and publications are available on Rafał's website (https://p.wz.pwr.edu.pl/~weron.rafal/).

Part V

Minisymposia

MS1 Mathematical models in a disease and epidemiological context
MS2 Minisymposium on topological data analysis
MS3 Minisymposium on non-Gaussian time series analysis for local damage detection
MS4 Current trends in portfolio risk assessment and management
MS5 Requirements, Tools and Applications in the Simulation of Fluid Technical Netwoks
MS6 Mathematics for Industry in Modelling: Microwaves, Vortices and Geometric Design
MS7 Mathematical Methods in Cardiology
MS8 Efficient numerical solutions of applied differential equations
MS9 EU-MATHS-IN: Success Stories of Mathematical Technologies in Societal Challenges and Industry
MS10 Computational mathematics for partial differential equations: theory and applications
MS11 Neural network-based numerical solution of ODEs and PDEs
MS12 Analysis and Numerics of port-Hamiltonian Systems
MS13 ECMI SIG: Mathematics for Big Data and Artificial Intelligence
MS14 ECMI SIG: Computational Methods for Finance and Energy Markets
MS15 Nordic-African collaboration in Applied & Industrial Mathematics in the Eastern Africa Region
MS16 Mathematics for the environment
MS17 ECMI SIG: Mathematics for the Digital Factory
MS18 Minisymposium on stochastic models for climate, finance and insurance data
MS19 Mathematics for Industry in the Netherlands: Trending Topics
MS20 Unraveling neural networks with structure-preserving computing
MS21 Modelling simulation and optimization in electrical engineering (MSOEE)
MS22 The Essence of Mathematics in Industry
MS23 Selected Aspects of Education in Applied Mathematics
MS24 Recent challenges in high-order accurate numerical methods for differential equations
MS25 Mathematical and physical modeling of single particle tracking experiments
MS26 Stochastic Modelling in Insurance and Reinsurance

MS 01

Title: Mathematical models in an disease and epidemiological context

Organizers: Wolfgang Bock, Thomas Götz

Abstract The last pandemic showed that Mathematical Modelling indeed is needed to help forecasting and shape structure for decision making. Mathematical models in the epidemic context are often following different hierarchies based on data, simulation runtime and the questions that the model should answer. In the last two years there have been a boost in those models. The mini-symposia should serve as a platform for different models for disease spread on different levels of detail and moreover strengthen and form new links in order to achieve pandemic preparedness. The talks will involve differential equation models, agent based models, interacting particle systems, Stochastic Partial Differential Equations or Statistical Models and Data Scientific approaches.

	Tuesday
Room	CR 10 AC
11:20-13:00	Chairperson: Thomas Götz
10:40-11:05	Isti Rodiah
11:05-11:30	Radomir Pestow
11:30-11:55	Tyll Krueger
11:55-12:20	Anna Fome
15:30-13:00	Chairperson: Thomas Götz
15:30-15:55	Lukas Bayer
15:55-16:20	Moritz Schäfer
16:20-16:45	Jean-Guy Caputo
16:45-17:10	Roland Pulch
17:20-18:35	Chairperson: Thomas Götz
17:20-17:45	Roger Petterson
17:45-18:10	Mary Joy Togonon
18:10-18:35	Evans Kiptoo Korir

GEMS - GERMAN EPIDEMIC MICRO-SIMULATION SYSTEM

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In 2020, the COVID-19 pandemic hit several countries hard, including Germany. Due to the rapid global spread, the need for models to evaluate (non-pharmaceutical) interventions efficiently and quickly became apparent.

Microsimulations such as agent-based models (ABM) can help to simulate and evaluate the heterogeneity of a population as well as measures at the level of individuals or their environment. For this purpose, the OPTIMAGENT consortium is building a model for the disease spread of various pathogens with a synthetic population based on census data in Germany.

In this talk we reflect the process of building the model within an interdisciplinary model consortium and first basic model, we investigate the spread and present our current results.

EPIDEMIC PROPAGATION ON A NETWORK: A SIMPLE MODEL

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We analyze an epidemic model on a network consisting of susceptible-infected equations at the nodes coupled by diffusion using a graph Laplacian. The model has few parameters enabling fitting to the data and the essential ingredient of importation of infected people; these features were particularly important for the COVID-19 epidemic. Using a complete graph describing the main airports on the planet, the model allowed us to predict the arrival of the COVID epidemic in Mexico in March 2020. It is also useful to evaluate deconfinement scenarios and prevent a so-called second wave. We introduce an epidemic criterion to describe the initial growth of the epidemic on the network. This growth is exponential and the exponent is the maximum eigenvalue of a matrix formed by the susceptibles and the graph Laplacian. Assuming vaccination reduces the susceptibles, we evaluate the most efficient strategy. Using matrix perturbation theory, we find that it is best to vaccinate uniformly the network. Assuming we can only vaccinate 2 or 3 vertices, an important question is which vertices do we choose? The analysis reveals that the best choice corresponds to vertices such that the fluctuating part of the vector of susceptibles is closest to the eigenvector corresponding to the largest eigenvalue. Numerical calculations on a seven vertex graph and a graph inspired from the rail map of France confirm these findings.

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ANALYSIS OF A COMPETITIVE RESPIRATORY DISEASE SYSTEM WITH QUARANTINE

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Respiratory diseases are among other infectious diseases of a public health concern [1]. Implementing measures, such as quarantine (where the individuals contacted the infected are removed from the rest of the population), is one approach to mitigating the spread of such diseases [2].

We study a SEIQR (susceptible-exposed-infectious-quarantined-recovered) deterministic epidemic model with a single host population and multiple strains (-c and -i) to account for two competitive diseases with quarantine effects. To model the role of quarantine and isolation efficacy in disease dynamics, we utilize a linear function. Further, we shed light on the standard endemic threshold and determine the conditions for extinction or coexistence with and without forming co-infection. Next, we show the dependence of the criticality based on specific parameters of the different pathogens.

We found that the disease-free equilibrium (DFE) of the single-strain model always exists and is globally asymptotically stable (GAS) if $\tilde{\mathcal{R}}_k^q \leq 1$, else, a stable endemic equilibrium. On top of that, the model has forward bifurcation at $\tilde{\mathcal{R}}_k^q = 1$. In the case of a two-strain model, the strain with a large reproduction number outcompetes the one with a smaller reproduction number. If the co-infected quarantine reproduction number is less than one, the infections of already infected individuals will die out, and co-infection will persist in the population otherwise. Further, we found the effectiveness of quarantine depends on some factors, including the disease's transmission rate, potential inputs provided by the respective authority, and the duration of the quarantine period. In particular, we observe that proper application of rules and regulations in the quarantine could result in less possibility of infection.

We note that the quarantine and isolation of exposed and infected individuals will reduce the number of secondary cases below one, consequently reducing the disease complications if the total number of people in the quarantine is at most the critical value. These findings have implications for the development and advancement of effective public health policies and strategies to combat respiratory diseases.

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SENSITIVITY ANALYSIS OF CONTACT-RELATED INTERVENTIONS FOR MODELING EPIDEMICS

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Mathematical models used to understand the spread patterns of infectious diseases such as influenza and coronavirus disease 2019 (COVID-19) are very complex. The transmission component of the models can be modeled in an age-dependent manner by introducing a population contact matrix that describes the contact rates between age groups. In epidemic modelling, subtle changes in parameters affect disease dynamics such as the baseline reproduction number and the structure of the epidemic curve. This problem can be studied through a sensitivity analysis approach to express the impact of a change in the mixing pattern, which could lead to planning an optimal NPI intervention strategy.

In this talk, we examine the sensitivity of contact matrix elements estimated in [1] to gain insight into the impact of changing social contact structure based on Latin Hypercube Sampling (LHS). The Partial Rank Correlation Coefficient (PRCC) method uses these sampled contacts to find out which elements are important to the model. We also investigate an approach to aggregate the PRCC values to obtain pairwise sensitivity analysis results. The application of the methodology is illustrated by analyzing a COVID-19 model from [2], and the results could support the decision makers during a pandemic.

Keywords: Sensitivity analysis, age-dependent epidemic model, social contact matrix, Latin hypercube sampling (LHS), Partial rank correlation coefficient (PRCC).

Acknowledgments The authors thank the National Laboratory for Health Security Program RRF-2.3.1-21-2022-00006 for support.

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STRUCTURAL RISK FACTORS IN EPIDEMIC DYNAMICS OF COVID-19

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There have been great differences in the epidemic dynamics of COVID-19 between the countries across the world but also within the countries of the European Union. The detailed causes of these differences are up to now only poorly understood and their clarification remains a challenging task for future research. Besides differences in the timeline of non-pharmaceutical interventions and their specific realisations it is likely that country specific structural risk factors are as well a major reason for the heterogeneity in the outcomes of the first two years of the COVID-19 epidemic. In this talk we discuss four major structural risk factors in detail: age profile, household structure, workplace structure and workplace related mobility. Finally we discuss the impact of structural risk factors for pandemic preparedness and give recommendations on how to adopt them into plans for epidemic control of future infectious diseases.

SOCIAL LEARNING DURING PANDEMICS

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We investigate the effects of social learning on the progression of pandemics. For this we extend an agent based realization of the standard SIR model with behavioral effects, which would be otherwise hard to capture by differential equations. In particular, agents can learn from their own experiences and that of others by observing actions and consequences (observational learning) as well by exchanging their beliefs with others (belief exchange). In addition the agents are influenced by a certain sample of mediated observations (i.e. media). We observe then how social learning in the form of observational learning and belief exchange modify the peak, duration and progress of pandemics. Finally, the effects of media bias on the pandemic and the welfare of the population are investigated.

EPIDEMIC MODELLING BY BIRTH-DEATH PROCESSES WITH SPATIAL SCALING

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Interpretation of for instance S, I, and R that appear in equations describing epidemics may not always be obvious. It can for instance be a matter of whether they describe the number or fraction of individuals in each compartment. It also raises a question of the meaning of the parameters in those equations. Here is an attempt to give a hopefully transparent description by considering a density dependent epidemic modeling of birth-death process type based on early works by Kurtz from the 1970s'. If the population size is not varying by time, the birth-death approach allows ODE-approximation for large populations and diffusion approximation for semilarge populations by scaling with respect to the population size, i.e. approximations for the fractions of each compartment can be obtained. Here assuming, somewhat unrealistic, spatial homogeneity of the population, a scaling is then instead with respect to area i.e. the number of individuals in each compartment per area is considered. This spatial scaling allows diffusion approximation for the fraction of individuals in each compartment for models with varying population size.

OPTIMAL CONTROL OF A DENGUE MODEL WITH TEMPORARY CROSS IMMUNITY

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The dynamics of infectious diseases is often described by SIR models, which represent systems of ordinary differential equations (ODEs) for unknown compartment densities of susceptible (S), infected (I) and recovered (R) individuals, see [1]. Concerning Dengue fever, four serotypes of the virus are distinguished. An infection by some Dengue serotype generates permanet immunity to it, but only temporary cross immunity to other serotypes. SIR models have been designed for this class of problems, see [2], for example.

We consider a model regarding two serotypes of the virus, which consists of 14 ODEs for 10 human compartments and 4 mosquito compartments. In [3], an optimal control problem was investigated using this system of ODEs, where the objective function included a time integral with the number of infected humans. A minimization was performed by actions to reduce the number of mosquitos. The costs of the actions were taken into account by a penalizing term in the objective function. Alternatively, we include only the integral of the number of infected humans in the objective function, while a limitation on the actions is imposed by an additional constraint in integral form. We examine both the direct approach and the indirect approach for a numerical solution of this optimal control problem. Results of corresponding computations are presented.

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SCENARIOS FOR THE SARS-COV-2 PANDEMIC 2023 IN GERMANY

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Introduction: In the past two years, an increased incidence of SARS-CoV-2 infection has always been observed during the fall/winter season. This is associated with an increased disease burden due to severe disease course, hospitalization, and death. Meanwhile, extensive vaccination campaigns against SARS-CoV-2 have been carried out. Therefore, it can be assumed that the current population is relatively well protected against severe SARS-CoV-2 infection. However, the emergence of new virus variants may continue to pose a challenge, for instance in 2022 when different subvariants of the Omicron variant triggered several waves of infections. Simulation studies are an established tool to better assess the range of possible pandemic developments in the coming months. Three modeling scenarios were developed for serious infectious diseases. Furthermore, we also integrated information from an adaptive population-based panel for monitoring the spread of epidemic diseases in Germany into the modeling scenarios.
Methods: Using a pandemic contact matrix, we developed a deterministic SEIRS model with some additional compartments [1]. In the model, we also included a seasonal index that corresponds to the pandemic data for 2020-2021. We used an ordinary differential equation (ODE) model and an adapted model incorporating population-based information to assess different scenarios.
Results: We show how disease transmission is dominantly due to the seasonal index for all scenarios. In scenario 1, we assume a new variant every month. Here, the simulation generates a new seasonal wave of infections for the upcoming fall/winter season. The model predicts that the previous peak hospitalization rate in the fall of 2022 will be significantly exceeded if proper precautions are not taken. In simulations that assume a very high seasonal impact in this scenario, this scenario becomes very unfavorable. The actual level of burden on the healthcare system depends on the characteristics of the virus and the preventive measures taken. In scenario 2, we assume a new variant every three months. In all likelihood, the number of hospital admissions could peak at a level similar to that seen during the wave in the fall of 2022. In scenario 3, we assume a new variant every six months. The peak number of hospitalizations in this wave is a few below that observed during the wave in the fall of 2022.
Discussion: The three simulated scenarios presented are considered likely in principle, but no probability of their occurrence can be given at this time. In our view, the modeling performed here suggests that continued timely and regional surveillance of the infection situation and monitoring of new SARS-CoV-2 variants would be useful.

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AN INTEGRO-DIFFERENTIAL MODEL FOR THE SPREAD OF DISEASES

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During the last three years, COVID–19 has shown that there is an increasing value in accurate models for the local and global spread of diseases, also giving advice to policy makers on how to deal with them. Country and region based statistics from many countries, e.g. Germany and Poland, show that regionally contained cases can spread throughout the country in a short period of time, especially during the " first wave" in spring and summer 2020. Lockdowns and other social restrictions were imposed as a result in order to contain the infection numbers, to relieve the strain on the health system, and reduce the amount of severely ill or dead. How the spread of infections can be explained and how well measures actually work is still an open or widely discussed question in many countries. In this talk, we aim to model the local spread of infections by an integro-differential model. Lockdowns and other measures are included in our model(s) by a control function, which can be optimised unter several assumptions and questions. On the one side, the aim is to contain the disease as much as possible, on the other side, attention has to be paid on the social and political costs of a lockdown, especially when case numbers are (comparatively) low, also taking into account not to overload the health capacities and other problems like Long COVID or economic problems given large infection numbers. A classical susceptible–infected–recovered (SIR) model is enhanced by an integral kernel (instead of the typical homogeneous mixing between susceptibles and infectives). We define several requirements on the kernel function and present several analytical findings of a reduced SIS and the applied SIR model. In the following, we define the required target function for the optimisation of the " lockdown" control and present the corresponding Forward-Backward method. Numerical results for various parameter choices are shown. In order to validate the numerical results of the integro-differential model, we compare them to those of an established agent–based model in which social factors can be inplemented more accurately.

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MATHEMATICAL MODELLING OF CELL MIGRATION WITH CHEMOTAXIS AND HAPTOTAXIS

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Cell migration processes are governed by chemo-attractive movement along tissue fibers (haptotaxis). To mathematically model such a process on the cellular level, cells are treated as interacting particles using Newton' s equations with suitable forces and potential. In this talk, we show that for the governing interaction potential to be the (truncated) Lennard-Jones potential and long-range chemo-attractive forces of Coulomb type, the existence of a Vlasov limit. The well-posedness of the dynamics will then be discussed with suitable assumptions on the considered potentials. The results generated will be strengthened by numerical simulations. Finally, we will give an outlook on coupling this model with a tumor growth model to obtain a surrogate model for cancer.

MS 02

Organizers: Paweł Dłotko, Michał Lipiński, Justyna Signerska-Rynkowska, Rafał Topolnicki

Abstract Topological Data Analysis (TDA) is a young branch of mathematics blooming rapidly in the last two decades. The slogan "Data has a shape, the shape has a meaning" captures the central idea of the field. The study of local relations between objects allows us to uncover the global patterns veiled in the data. TDA provides a number of both qualitative and quantitative tools for data exploration, revealing features of data inaccessible through standard statistical methods. The potential of the topological approach led to a vast range of applications, both on theoretical and applied topics, e.g.: statistics, dynamical systems, scientific computations, neuroscience, material sciences, visualization, computer vision, and much more. Recently, the community's increased interest in relations between TDA and Machine Learning (ML) sparked many studies ranging from the applicability of topological features in ML to the explainability of ML methods using TDA. The workshop aims to gather researchers interested in Topological Data Analysis and those seeking new mathematical ideas on how to explore their data.

	Monday
Room	CR 10 B
10:40-11:05	Paweł Dłotko
11:05-11:30	Frank Lutz
11:55-12:20	Mathijs Wintraecken
11:55-12:20	Andrea Guidolin
15:30-15:55	Julian Brüggemann
15:55-16:20	Francesca Tombari
16:20-16:45	Justyna Signerska-Rynkowska
16:45-17:10	Michał Lipiński

	Tuesday
Room	CR 114
10:40-11:05	Rafał Topolnicki
11:05-11:30	Sara Scaramuccia
11:30-11:55	Niklas Hellmer

ON THE SPACE OF DISCRETE MORSE FUNCTIONS

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Discrete Morse Theory is a versatile tool to analyze regular CW complexes and, in particular, simplicial complexes in many contexts. It has applications in both pure and applied mathematics.

After a brief introduction to discrete Morse theory, we are going to analyze the structure of the space of discrete Morse functions on a given simplicial complex X. It turns out that its topological properties are subject to an oriented hyperplane arrangement induced by the face poset of X and the definition of discrete Morse functions as given by Forman [1]. We are going to look into a couple of basic properties of the space of discrete Morse functions and, if time permits, we will consider how this point of view allows us to understand the space of merge trees as a quotient of the space of discrete Morse functions.

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TOPOLOGICAL VISUALIZATION METHODS

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In this talk I will present a number of Topological Data Analysis-originated visualization methods. In particular, I will discuss mapper and ball mapper algorithms along with recent cluster graph algorithms. A number of use cases of those techniques will be shown.

Acknowledgments P.D. acknowledges support by Dioscuri program initiated by the Max Planck Society, jointly managed with the National Science Centre (Poland), and mutually funded by the Polish Ministry of Science and Higher Education and the German Federal Ministry of Education and Research.

STABLE HOMOLOGICAL INVARIANTS OF DATA FROM ALGEBRAIC WASSERSTEIN DISTANCES

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Distances to compare data representations or their invariants play a fundamental role in Topological Data Analysis. Via a technique called hierarchical stabilization, a choice of a pseudometric between persistence modules yields an associated stable homological invariant. In applications, considering rich families of pseudometrics is often advantageous, as meaningful pseudometrics may depend on the task at hand.

We introduce a parametrized family of pseudometrics between persistence modules based on the algebraic Wasserstein distance defined by Skraba and Turner [1], and phrase them in the formalism of noise systems [2]. These pseudometrics are used to define associated stable invariants, called Wasserstein stable ranks, which can be computed efficiently. We illustrate the advantages and the versatility of our framework for data analysis based on Wasserstein stable ranks both on artificial and real-world data. A preprint of the work is available [3].

Acknowledgments This work was partially supported by the Swedish Research Council (Vetenskapsrådet) and the Wallenberg AI, Autonomous Systems and Software Program (WASP) funded by the Knut and Alice Wallenberg Foundation.

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DAMAGE IDENTIFICATION IN ROLLING ELEMENT BEARINGS USING TOPOLOGICAL DATA ANALYSIS

Niklas Hellmer[a], **Justyna Hebda-Sobkowicz**[b], **Radosław Zimroz**[b], **Agnieszka Wyłomańska**[c] and **Paweł Dłotko**[a]

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Detection of periodic/cyclic impulses p embedded in an unknown signal s is a considerable challenge. Typically s is nondeterministic noise sampled from an unknown, often non-Gaussian distribution. In this work, we adopt the tools of topological data analysis to analyze signal $s + p$ and to determine existence of nonzero component p in the signal. This approach is agnostic to the model generating s and p. It is based on Takens' reconstruction theorem and uses persistent homology based methods to detect subtle changes in dynamics generating the signal $p+s$. Consequently it allows detection of the existence of periodic component p given a sample of signals s in which such component is not present.

DYNAMICS RECONSTRUCTION FROM A TIME SERIES

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In this talk we present a few developed tools that together form a pipeline for the reconstruction of dynamical system properties from a finite time series. The first step involves Takens' embedding technique and embedding dimension estimation to unwrap the underlying phase space. Then, a manifold reconstruction with the Patched Witness Complex allows us to construct a simplicial approximation of an attractor. On top of the obtained simplicial complex, we build a combinatorial multivector field guided by the time series. Finally, the combinatorial dynamical system can be further analyzed by detecting isolated invariant sets, or globally characterized by finding a Morse predecomposition of the system.

TOPOLOGICAL MODELLING OF METALLIC FOAMS

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Understanding material' s microstructure is key to link inner structure information to large-scale physical properties and function. An improvement of the microstructure during production processes can lead to materials with enhanced physical properties or even to the development of new classes of materials.
In this talk, we focus on metallic foams, in particular, on Al-alloy based foams that are produced by inserting air bubbles (by blowing in air or by a chemical reaction) into a metallic liquid that is solidified over the process. The resulting material then consists of a metallic framework that contains voids.
In the physics literature, such wet foams are usually modelled by replacing each (typically non-convex) foam bubble by a round ball of the same volume for which then their Laguerre–Voronoi diagram is computed.
In an approach to better capture the non-convexity of the foam bubbles, we rely on the combinatorial part of Plateau' s rules for dry foams that four bubbles jointly meet to form a vertex of a dual triangulation and three bubbles lie around each edge of the dual triangulation. In our modelling, we allow parallel edges as well as multiple triangles and tetrahedra as simplices of a generalized triangulation—dual to a simple decomposition of the foam that replaces the standard Laguerre–Voronoi diagram.

PARALLEL DECOMPOSITION OF PERSISTENCE MODULES THROUGH INTERVAL BASES

Alessandro De Gregorio[a], **Marco Guerra**[a], **Sara Scaramuccia**[b] and **Francesco Vaccarino**[a]

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In most applications of topological data analysis, computing persistent homology is normally limited to obtaining the persistence pairs, possibly with their associated cycle representatives. The corresponding persistence module is then identified up to isomorphism, but its explicit decomposition is avoided by common algorithms. Here, we leverage the persistence module representation as a graded module to introduce an interval basis, i.e. a special system of generators that are kept independent along the graded structure which provide an explicit persistence module decomposition at algebraic level. Generators obtained via standard algorithms for persistence do not necessarily form an interval basis. We introduce and compare two algorithms for the interval basis computation, one specialized from a graded version of the Smith normal form, and a new parallel one. In the final part, we focus on some possible applications of interval bases in locating cycle representatives and investigating functorial properties.

DYNAMICS RECONSTRUCTION FROM FINITE SAMPLE

Justyna Signerska-Rynkowska[a,b], **Paweł Dłotko**[a] and **Michał Lipiński**[a,c]

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Given two time series, we consider the problem of assessing the similarity of the underlying dynamical (deterministic) processes which generate them. In the theory of dynamical systems the equivalence between two systems is expressed using a notion of topological conjugacy. We show how this purely mathematical idea can be used for assessing the similarity of the two dynamical processes in a situation when only (finite) time-series generated by them are attainable. Precisely, given $x_1, \ldots, x_n \subset X$ and $y_1, \ldots, y_n \subset Y$ as well as $h : X \to Y$, and assuming that $x_{i+1} = f(x_i)$ and $y_{i+1} = g(y_i)$ for some deterministic systems (X, f) and (Y, g), we deliver a number of tests to check if f and g are topologically conjugated via h. The values of the tests are close to zero for conjugated systems and large for systems that are not conjugated. The method also applies to the situation when one has measurements of two observables of deterministic processes, of a form of one or higher dimensional time-series since their similarity can be accessed by comparing the dynamics of their Takens' reconstructions. We provide examples indicating scalability and robustness of the methods.

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GEOMETRY OF THE MATCHING DISTANCE FOR 2D FILTERING FUNCTIONS

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The matching distance is a metric studied in multiparameter persistence theory. Its computation, in the context of biparameter persistence, has produced several successful efforts turning into more and more efficient algorithms. In this talk, we will explore the geometry of the matching distance and its dependence on the differential structure of the filtering functions from which the persistence invariants are extracted. We will introduce the extended Pareto grid associated with a smooth function from a closed Riemannian manifold to the real plane, explain how this grid can be used to find persistence features and use this information to deepen our understanding of the matching distance. This talk is based on [1].

References

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APPLICATION OF TOPOLOGICAL DATA ANALYSIS TO GOODNESS-OF-FIT TESTING

Rafał Topolnicki, **Niklas Hellmer**, **Paweł Dłotko**, and **Łukasz Stettner**

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In the talk a novel application of topology to statistical hypothesis testing will be presented [1]. A new approach, driven by concepts originating in Topological Data Analysis, to multivariate one- and two-sample goodness-of-fit tests will be discussed. The presented tests work for samples in arbitrary dimensions, having comparable power to the state-of-the-art tests in the one-dimensional case. It is demonstrated that the type I error can be controlled and their type II error vanishes with increasing sample size. Derived theoretical results will be discussed and the finite-sample performance will be addressed by extensive numerical conducted to demonstrate their finite sample power.

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TIGHT BOUNDS FOR THE LEARNING OF HOMOTOPY À LA NIYOGI, SMALE, AND WEINBERGER FOR SUBSETS OF EUCLIDEAN SPACES AND OF RIEMANNIAN MANIFOLDS

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In this talk we extend and strengthen the seminal work by Niyogi, Smale, and Weinberger[1] on the learning of the homotopy type from a sample of an underlying space. In their work, Niyogi, Smale, and Weinberger studied samples of C^2 manifolds with positive reach embedded in $\mathbb{R}^d$. We extend their results in the following ways: In the first part of our paper we consider both manifolds of positive reach — a more general setting than C^2 manifolds — and sets of positive reach embedded in $\mathbb{R}^d$. The sample P of such a set $\mathcal{S}$ does not have to lie directly on it. Instead, we assume that the two one-sided Hausdorff distances — ε and δ — between P and $\mathcal{S}$ are bounded. We provide explicit bounds in terms of ε and δ, that guarantee that there exists a parameter r such that the union of balls of radius r centred at the sample P deformation-retracts to $\mathcal{S}$. To be more concrete:

- We provide tight bounds on ε and δ for sets of positive reach. We exhibit their tightness by an explicit construction.
- We also provide tight bounds in the case where the set $\mathcal{S}$ is a manifold, thus improving the bounds given by Niyogi, Smale, and Weinberger. Again, we prove the tightness of the bounds by constructing explicit examples.
- We simplify Niyogi, Smale, and Weinberger's proof using Federer's work on the reach, and several geometric observations. It is thanks to the streamlined proof that we can easily extend the reconstruction from C^2 manifolds to sets of positive reach. We also carefully distinguish the roles of δ and ε, which is essential to achieve tight bounds. The separation of δ and ε is sensible in practical situations, where the noise is generally much smaller than the sample density.

If time allows we'll consider homotopy learning in a significantly more general setting — we investigate sets of positive reach and submanifolds of positive reach embedded in a *Riemannian manifold with bounded sectional curvature*. To this end we introduce

a new version of the reach in the Riemannian setting inspired by the cut locus. Yet again, we provide tight bounds on ε and δ for both cases (submanifolds as well as sets of positive reach), exhibiting the tightness by an explicit construction.

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MS 03

Organizers: Agnieszka Wyłomańska, Radosław Zimroz

Abstract The vibration-based local damage detection is related to the identification of cyclic and impulsive behavior in the analyzed signal. The component of the signal with such property is called the signal of interest. Most of the classical methods are based on the strong assumption of finite-variance distribution of the underlying data. The most common distribution with a such property is the Gaussian one. However, in real environment the measured signals very often exhibit non-Gaussian characteristics that are manifested by large observations in the analyzed vectors. Thus, in the recent years new approaches for local damage detection appeared in the literature and advanced mathematical methods taking into account the possible large observations were proposed. The speakers will demonstrate the new achievements in the area of local damage detection for the non- Gaussian and non-stationary signals. The minisymposium aims to gather researchers interested in new mathematical ideas on how to analyze the non-Gaussian distributed data for identification of the signal of interest.

	Friday
Room	CR 115
10:40-11:05	Wojciech Żuławiński
11:05-11:30	Mateusz Gabor
11:55-12:20	Jacek Wodecki
11:55-12:20	Hubert Woszczek
15:30-15:55	Agnieszka Wyłomańska
15:55-16:20	Katarzyna Skowronek
16:20-16:45	Justyna Witulska

NONNEGATIVE TENSOR FACTORIZATION WITH β-DIVERGENCE COST FUNCTIONS FOR VIBRATION-BASED LOCAL DAMAGE DETECTION

Mateusz Gabor[a] , **Rafal Zdunek**[a] , **Radoslaw Zimroz**[b] , **Jacek Wodecki**[b] and **Agnieszka Wyłomańska**[c]

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The vibrational signals from the faulty machine are non-stationary, hence there is a need to use the time-frequency representations to analyze such signals. The most common time-frequency representation is a spectrogram. Because the magnitude part of the spectrogram is a non-negative matrix, it can be decomposed using the non-negative matrix factorization (NMF). NMF decomposes the spectrogram of the input signal into two separate matrices that contain the frequency and temporal features of the input signal. Such a decomposition works as a blind source separation method, which separates the signal of interest (SOI) of the input mixture of sources from the background noise. Recently, NMF has been used for local damage detection in bearings, but was limited to minimization of the Euclidean cost function. In this study, we extended the idea of using NMF for local damage detection, introducing the non-negative tensor factorization (NTF) model, which generalizes the NMF model by decomposing the set of stacked spectrograms. Furthermore, the β-divergence cost functions were used for both the NMF and NTF models. The Euclidean cost function has few limitations and does not perform well on spectrograms, the other cost functions from the β-divergence family such as Kullback-Leibler and Itakura- Saito perform better. Experiments carried out with synthetic and real signals show the high efficiency of the proposed method compared to the NMF approach.

Acknowledgments The work is supported by National Center of Science under Sheng2 project No. UMO-2021/40/Q/ST8/00024 " NonGauMech - New methods of processing non-stationary signals (identification, segmentation, extraction, modeling) with non-Gaussian characteristics for the purpose of monitoring complex mechanical structures" .

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IDENTIFICATION OF THE NOISE COMPONENT PROPERTIES IN TIME-FREQUENCY DOMAIN WITH APPLICATION TO VIBRATION SIGNALS ANALYSIS

Katarzyna Skowronek[a], **Tomasz Barszcz**[b], **Jérôme Antoni**[c], **Radosław Zimroz**[d] and **Agnieszka Wyłomańska**[a]

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Condition monitoring relates to detection of signal of interest (SOI) in presence of the disturbing noise. The commonly used diagnostic procedures assume Gaussian distribution of the background noise. However, it might not always be the case since in many situations the SOI may be hidden in highly impulsive, non-Gaussian noise. In some cases, the distribution of the background noise may have infinite variance which prevents from using classical methods, such as autocorrelation function (ACF), to detect SOI. Hence, it is important to assess the properties of the noise in the signal. In this work, we present a novel test procedure to identify the non-Gaussian behaviour in time-frequency domain. Our approach is based on estimating the empirical cumulative even moments (ECEM) in time-frequency representation of the input signal and comparing empirical statistics with the same statistics obtained for Gaussian noise transformed into time-frequency domain. In our analysis, we consider presented methodology for both simulated signals and real vibration data obtained from various machines.

Acknowledgments The work is supported by National Center of Science under Sheng2 project No. UMO-2021/40/Q/ST8/00024 "NonGauMech - New methods of processing non-stationary signals (identification, segmentation, extraction, modeling) with non-Gaussian characteristics for the purpose of monitoring complex mechanical structures".

References

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MULTIDIMENSIONAL PREDICTIVE MODELING FOR 5G NETWORK DIMENSIONING

Justyna Witulska[a], **Dominik Dulas**[b,c], **Ireneusz Jabłoński**[c,d], and **Agnieszka Wyłomańska**[a]

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The main goal of this research is to design a predictive model dedicated to 5G network dimensioning. Dimensioning the 5G network is a significant task from the point of view of ICT network management [1]. Appropriate network management allows 5G network operators to provide services at the highest level. Inadequate allocation of resources means that the operator may incur costs of breaking contracts with the customer (underestimation) or incur losses related to providing more resources than the actual demand (overestimation) [2]. We focus on the development of multidimensional time series models [3] and neural networks [4] that allows us to predict two variables: delay and throughput. We suggest utilizing Principal Component Analysis for multivariate time series to reduce the time of fitting the model to the data. In the case of neural networks, we propose an approach based on signal decomposition and prediction of its components. We use structures based on convolutional networks, LSTM, bidirectional LSTM, and GRU. The models are applied to the data registered in the network's operator. Correlation analysis justifies the use of multivariate predictive models. Models are validated using the following measures: MAE, RMSE, MAPE.

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FACTORIZATION OF MULTIDIMENSIONAL DATA STRUCTURES AS A TOOL FOR DECOMPOSITION IN NONSTATIONARY SCENARIOS FOR VIBRATION-BASED CONDITION MONITORING

Jacek Wodecki[a], **Anna Michalak**[a], **Agnieszka Wyłomańska**[b] and **Radosław Zimroz**[a]

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Local damage detection in rotating machine elements is still a very important problem widely researched in the literature. One of the most common approaches is vibration signal analysis. Since time-domain processing is often insufficient, multidimensional representations are frequently favored. Commonly used ones include time-frequency representations (i.e. Short-Time Fourier Transform), cyclostationary maps (i.e. Cyclic Spectral Coherence), and many others [1,2]. Factorizing such representations can be beneficial for the separation of internal processes occurring in the data. Since many of such representations are inherently nonnegative, it is proposed to use the approach of Nonnegative Matrix Factorization (NMF) for decomposition of such structures [3]. In this talk authors present several approaches to use the products of such factorization for extracting informative features, which leads to reconstruction and evaluation of internal data components.

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AUTOREGRESSIVE MODEL WITH DOUBLE PARETO DISTRIBUTED NOISE

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Time series models are a popular tool commonly used to describe time-varying phenomena. One of the most popular models is the Gaussian autoregressive (AR) model. However, when the data has observations with possible large values, Gaussian models are not a good choice. We therefore abandon the assumption of normality of the data distribution and propose the AR model based on the double Pareto distribution. We introduce the estimating algorithm for the model's parameters, obtained by the maximum likelihood method. For this purpose, we use the Maclaurin series expansion and the Chebyshev polynomials expansion of the likelihood function. We compare the results with the Yule-Walker estimator in the finite-variance case and with the modified Yule-Walker estimator in the infnite-variance case. The efficiency of the results obtained was checked by Monte Carlo simulations.

THE IMPORTANT ROLE OF BACKGROUND NOISE PROPERTIES FOR SELECTION OF TOOLS FOR LOCAL DAMAGE DETECTION

Agnieszka Wyłomańska[a], **Katarzyna Skowronek**[a], **Jérôme Antoni**[b], **Radosław Zimroz**[c]

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Any measured diagnostic signal is associated with noise disturbance. To date, most diagnostic procedures have assumed a Gaussian distribution of noise. We give a new perspective on the problem of local damage detection and show that background noise distribution properties determine tools for signal analysis. Thus, the recognition and identification of possible non-Gaussian behaviour of the noise is of great importance. We emphasise the important role of variance, as most signal analysis methods are based on the assumption of a finite probability distribution of the underlying signal. The problem is shown using three commonly observed non-Gaussian distributions for real vibration signals. We show how the properties of the noise in the time domain can change when transformed into time-frequency domains (spectrograms).

Acknowledgments The work is supported by National Center of Science under Sheng2 project No. UMO-2021/40/Q/ST8/00024 "NonGauMech - New methods of processing non-stationary signals (identification, segmentation, extraction, modeling) with non-Gaussian characteristics for the purpose of monitoring complex mechanical structures".

ROBUST STATISTICS IN APPLICATION TO PERIODICITY DETECTION FOR NON-GAUSSIAN SIGNALS - ANALYSIS IN TIME-FREQUENCY AND FREQUENCY-FREQUENCY DOMAINS

Wojciech Żuławiński[a], **Aleksandra Rogalska**[a], **Jérôme Antoni**[b], **Radosław Zimroz**[c] and **Agnieszka Wyłomańska**[a]

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Many local damage detection procedures are based on the periodicity detection methods. One can analyze a signal in this context in the time and frequency domains. In both of them, the utilized methodologies use the autocorrelation (ACF) measure and its standard estimator called sample ACF. This approach is very efficient if the distribution of the analyzed signal's background noise is Gaussian (or close to Gaussian). However, in some situations, it might not be the case. Instead, the considered signal of interest might be disturbed by strongly impulsive non-Gaussian noise. In such cases, the standard methods might not be able to correctly extract the information about periodicity. It is caused by the fact that the sample ACF is not resistant to significantly outlying values. Hence, for signals with the described non-Gaussian behaviour, we propose to use robust ACF estimators which are much less sensitive to outliers. In this work, we consider trimm, Kendall and Spearman estimators, although this approach is much more general and other robust methods can also be used. We apply robust ACF estimators for the periodicity detection methods in the time-frequency (i.e. spectrogram-based autocorrelation maps) and frequency-frequency domains (i.e. spectral coherence maps). The presented methodologies are applied to the simulated signals (considering three types of non-Gaussian distribution) and to the real vibration dataset from the crushing machine.

Acknowledgments The work is supported by National Center of Science under Sheng2 project No. UMO-2021/40/Q/ST8/00024 "NonGauMech - New methods of processing non-stationary signals (identification, segmentation, extraction, modeling) with non-Gaussian characteristics for the purpose of monitoring complex mechanical structures".

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MS 04

Organizers: Burcu Aydogan, Mervan Aksu

Abstract During the global pandemic, almost all central banks went to monetary expansions. The effects of these expansions make the financial system to be more volatile and fragile. In other words, those effects make the financial markets more risky. This leads all parties in finance to be more aware of the risk assessment and management. In finance literature, identification and investigation of risk factors have been become more popular especially after pandemic.
In this symposium, we want to address the risk assessment and management which have been always crucial issues in decision making for combined assets of an investor. During the volatile market conditions, one of the most important challenges for an investor is the portfolio risk in which the investor needs to assess and manage the risk by identifying and analyzing the types of risk faced with. There are two types of risks associated with building a secure portfolio: systemic risk and unsystemic risk. The risk can be figured out by the well- known metrics such as standard deviation, Sharpe ratio, beta and Value at Risk (VaR) which can be combined with machine learning, artificial intelligence and deep neural networks. These recent techniques lead to more dynamic risk management strategies where the portfolio' s risk profile is actively tracked and adaptations are handled depending on the updated profiles. Our aim is to learn about the new techniques in order to contribute to the literature on the innovative approaches of the risk metrics estimation.

	Monday
Room	CR 113
10:40-11:05	Burcu Aydogan
11:05-11:30	Mogens Steffensen

OPTIMAL INVESTMENT STRATEGIES UNDER THE RELATIVE PERFORMANCE IN JUMP-DIFFUSION MARKETS

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We work on a portfolio management problem for a representative agent and a group of people, forming a market under relative performance concerns in a continuous-time setting. Herein, we define two wealth dynamics: the agent' s and the market' s wealth. The wealth dynamics appear in jump-diffusion markets. In our setting, we measure the performances of the market and the individual agent with preferences linked to the market performance. Therefore, we have two classical Merton problems to determine what the market does and the agent' s optimal strategy relative to the market performance. Furthermore, our framework assumes that the agent' s utility performance does not affect the market, while the market affects the agent' s utility. We explore the optimal investment strategies for both the agent and the market.

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OPTIMAL CONSUMPTION, INVESTMENT, AND INSURANCE UNDER STATE-DEPENDENT RISK AVERSION

Mogens Steffensen and **Julie Bjørner Søe**

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We formalize a consumption-investment-insurance problem with the distinction of a state-dependent relative risk aversion. The state-dependence refers to the state of the finite state Markov chain that also formalizes insurable risks such as health and lifetime uncertainty. We derive and analyze the implicit solution to the problem, compare it with special cases in the literature, and illustrate the range of results in a disability model where the relative risk aversion is preserved, decreases, or increases upon disability.

MS 05

Organizers: Gerd Steinebach, Michael Hilden

Abstract Technical fluid networks from the areas of hydraulic braking systems, hydrogen storage, sector coupling, drinking water supply and gas pipelines are considered. The reliable and meaningful simulation requires the detailed modelling of individual components up to the consideration of large-scale areas over longer periods of time. The aim is to provide a model family with different abstraction levels for these tasks. In the mini-symposium, various aspects will be examined in more detail. The tool chain used ranges from suitable measurement methods via FE detailed models, parameterised component models up to one-dimensional pipe networks and the sector coupling electricity-gas-heat. In addition, aspects of implementation, the further development of DAE solvers and metamodeling by radial basis functions are discussed.

	Thursday
Room	CR 113
10:20-10:45	Michael Hilden
10:45-11:10	Gerd Steinebach
11:10-11:35	Michael Bareev-Rudy
11:35-12:00	Tanja Clees

OPTIMAL SIZING AND CONTROL OF A HYDROGEN-BASED HYBRID ENERGY STORAGE SYSTEM BY MEANS OF METAMODELING

Michael Bareev-Rudy[a], **Gerd Steinebach**[a] and **Tanja Clees**[a,b]

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To mitigate the effects of climate change, energy production must rapidly shift from fossil fuels to renewable sources. Due to the intermittent nature of renewable energy sources such as PV and wind, energy storage is required.

One promising component to enhance Power-to-Gas-to-X (PtGtX) systems is hydrogen storage. Hydrogen is produced with an electrolyzer, stored (e.g.) in a metal hydride reservoir, and can be converted back to electricity with a fuel cell when needed. In combination with a buffer battery, such a storage system is called a Hybrid Energy Storage System (HESS). Such a system can be considered in different scenarios, e.g. isolated as an island system or integrated into electricity and gas networks. By using electricity, hydrogen and heat, such a system is also suitable for sector coupling.

In this work, a PtGtX system with a HESS is investigated for optimal control and sizing of its components for different application scenarios. For this purpose, such a system at the H-BRS is simulated in a self-developed, object-oriented Multiphysical Energy System Simulator (MEgy) [1]. In order to investigate the behavior of the simulation model in different scenarios, the parameters are varied based on a space-filling sampling plan. The simulation results are evaluated according to application-specific criteria and used to build a meta-model based on radial basis functions with polynomial detrending. This in turn is used by optimization algorithms to find the optimal sizing for a given scenario.

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CONTINGENCY ANALYSIS FOR GAS TRANSPORT NETWORKS WITH HYDROGEN INJECTION

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Hydrogen plays a growing role in approaches for transforming the overall energy system. In particular, power-to-gas (PtG) plants, which can convert electrical power to hydrogen by means of electrolysis, are considered as an important ingredient for employing excess power from renewable ressources. Hydrogen might be injected to existing networks for transport of natural gas, or separate hydrogen networks can be used. However, such approaches need intense planning and optimization based on simulations for several reasons. One of these impacts might be less security. Hence, intense contingency analysis should be performed to estimate locations of probable failures and magnitudes of additional capacity needed.

Contingency analysis is widely used for electrical networks. A so-called $N-1$ analysis is standard. For gas transport networks or coupled networks, a comparable analysis can be performed, but is not standard.

Adapted $N-1$ analysis methods as well as an analysis of multi-element contingencies, based on so-called supernodes, are introduced in [1]. They are based on ensemble simulations.

In this talk, an extension of these methods by means of numerical optimization for the placement and capacity of hydrogen storage facilities is introduced. The efficiency of the overall method is demonstrated for a realistic gas transport network model.

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CHALLENGES IN BRAKE FLUID NETWORKS MEASUREMENTS & SIMULATIONS

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Passenger cars and light commercial vehicles are typically equipped with hydraulic brake systems. The hydraulic medium "brake fluid" transmits and converts the braking force from the driver's brake pedal in the brake master cylinder into hydraulic pressure, which is routed via brake lines in the vehicle network to the wheel brake and there converted back into braking force.

Vehicle-dynamics control systems such as the antilock braking system or the electronic stability program can additionally modulate the hydraulic pressures at each wheel to prevent the wheels from locking through pressure reductions or to stabilize the handling through additional pressure build-ups.

The medium "brake fluid" needs to be a "reliable fluid", i.e., to be "reliable" as compatible within the network (low corrosion with metals, oxidation, EPDM sealing swelling) and to stay "fluid-incompressible" in the complete operating temperature range without vapor lock risks and soft brake issues.

Future trends require a minimum lubrication performance to avoid challenges noise and wear in product use ensured by developed standardized tribometer tests [1,2]. Finally, air solubility can provoke outgassing of dissolved air with "soft brake" issues to be avoided.

Different required mathematical details are applied for challenges in "brake fluid networks" measurements & simulations. These consist of data analysis sigma method as oscillation occurrence measure, FEM models with dynamic friction approach [3] or filter stabilization of data differentiations.

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SIMULATION OF ENERGY NETWORKS WITHIN JULIA APPLICATIONS AND BENCHMARKS WITH METHOD RODAS5P

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For a successful energy transition, coupled networks of the gas, heat and electricity sectors with suitable storage options are needed. Mathematical models of these networks allow scenario calculations over longer periods of time and support the design and dimensioning of storage capacities.

In this paper, we therefore first deal with the modeling of multiphysics networks consisting of coupled fluid flow elements and other components. For the solution of the resulting differential-algebraic equation systems fast and robust methods are needed. With the package DifferentialEquations.jl Julia offers a very comprehensive selection of methods. Furthermore, the programming language Julia is freely available, relatively easy to learn and very performant.

Using suitable benchmarks, we can show that the new method Rodas5P is a good candidate for the energy network simulator. We go into the construction and the properties of the method, which belongs to the family of Rosenbrock-Wanner methods that have already been successfully used in similar applications concerning water and gas flow [1,2].

Finally, we discuss some practical examples and show by numerical tests that the chosen approach is well suited for the presented simulation tasks.

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MS 06

Organizers: Kenji Kajiwara, Yasuhide Fukumoto, Mark McGuiness, Yoshiki Jikumaru

Abstract Mathematics for Industry (MfI) aims at developing a new research area of mathematics by responding to the needs of the industry and society by reorganizing pure and applied mathematics into flexible and versatile forms. In this minisymposium four talks on specific emerging MfI by the delegates of the Asia Pacific Consortium of Mathematics for Industry will be given, with the topics on mathematical modelling of various settings: microwaves transmission, vortex pair dynamics, structure modelling and geometric aesthetic shape design.

	Monday
Room	CR 10 D
10:40-11:05	Mark McGuinness
11:05-11:30	Yasuhide Fukumoto
11:30-11:55	Yoshiki Jikumaru
11:55-12:20	Kenji Kajiwara

GLOBAL TIME EVOLUTION OF A VORTEX PAIR IN A VISCOUS FLUID

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Vortex pairs act to produce lift and thrust of aircrafts and animals. They move by themselves, entraining surrounding fluid, and are capable of transporting neutrally buoyant materials over long distances. We develop a method for calculating self-induced motion of a counter-rotating vortex pair over the entire time range, including the decaying stage, with focus on the influence of viscosity.

Initial-value problems are solved for a vortex pair embedded in a viscous fluid. For high-Reynolds-number motion, the method of matched asymptotic expansions in powers of the ratio of the core radius to the distance between vortices, a small parameter, is used to derive the traveling speed of the pair at early times [1]. This gives the upper bound on the traveling speed in an early stage. As an alternative means, we adapt, to the two-dimensional vortical flow, Helmholtz-Lamb's formula for an axisymmetric vortex ring. This method saves, to a large extent, manipulations of asymptotic expansions. In the large-Reynolds-number limit, a topological method (Kelvin-Benjamin's kinematic variational principle) achieves a further simplification (*cf.* [2], [3]).

For low-Reynolds-number motion, the vorticity obeying the Stokes equation is substituted into the 2D-version of Helmholtz-Lamb's formula. At early times, this gives the lower bound on the traveling speed. An analysis at large times reveals the decaying behavior of the traveling speed, being distinct from the axisymmetric case [4].

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ON THE APPLICABILITY OF DISCRETE CONFORMAL MAPS TO TRUSS STRUCTURES IN ARCHITECTURAL DESIGN

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A classical truss structure discovered by A. G. M. Michell [1] is known as one that efficiently transmits loads with a minimum number of possible members. In this talk, we discuss a truss structure analogous to the Michell truss constructed by the method of discrete differential geometry [2]. We show that our proposed structure has nice mechanical properties and constructibility and a deep connection with log-aesthetic curves [3], [4].

Acknowledgments The authors are grateful for the support of the Scientific Fund (Joint Research Center for Advanced and Fundamental Mathematics-for-Industry Grant No. 2022a034).

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GENERATION OF AESTHETIC CURVES AND SURFACES BY INTEGRABLE GEOMETRY

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We consider some generalizations of a family of plane curves called the log-aesthetic curves (LAC) developed and used in industrial design as shape elements with built-in aesthetic nature. Under the framework of similarity geometry, LAC is shown to be analogue of Euler' s elastica in Euclidean geometry. Based on this characterization we propose generalization of LAC to space curves and surfaces with the aid of integrable geometry.

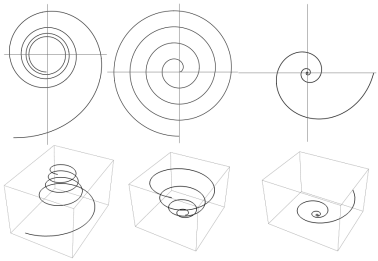

Figure1. Typical LACs and 3D extensions: Clothoid, Circle Involute and Logarithmic Spiral.

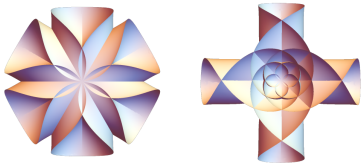

Figure2. Similarity geometry analogue of pseudo- spherical surfaces.

Acknowledgments The authors are grateful for the support of JSPS Kakenhi JP21K03329 and JST CREST Grant Number JPMJCR191.

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MODELLING MOISTURE DETECTION IN BAUXITE USING MICROWAVES

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An ESGI problem from 2017 presented us with challenging data for the phase shift and signal strength seen in microwaves travelling through bauxite ore on a conveyor belt. The data comes from an automated real-time moisture detector used in an alumina factory, and shows serious inconsistencies with a semi-infinite linear model that underlies the operation of the detector. A four-layer model based on Maxwell's equations provides better agreement with data, and some answers about the role played by reflections and interference of travelling microwaves at interfaces.

MS 07

Organizers: Grzegorz Graff, Ulrich Parlitz

Abstract During last years many new mathematical methods have been developed and successfully used in various branches of medical research. The minisymposium will be an interdisciplinary forum for discussion about wide range of topics related to applications of mathematical tools in cardiology. The session will cover among other issues the following topics: nonlinear and statistical methods in cardiovascular research, mathematical analysis of cardiorespiratory interactions, dynamic impedance cardiography, models describing complex excitation patterns in the myocardium underlying cardiac arrhythmias, machine learning methods for data-driven modeling of cardiac dynamics, and clinical applications of mathematical methods.

	Tuesday
Room	CR 113
10:40-11:05	Gerard Cybulski
11:05-11:30	Sebastian Herzog
11:55-12:20	Sayedeh Hussaini
11:55-12:20	Monika Petelczyc
15:30-15:55	Teodor Buchner
15:55-16:20	Katarzyna Kubiak
16:20-16:45	Katarzyna Tessmer
16:45-17:10	Grzegorz Graff

FROM ECG TO ENERGY STORAGE: UNIVERSALITY OF IMPEDANCE AND LACK OF KINETIC THEORY

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From the mathematical point of view, the source of an ECG signal is a series of discrete, stochastic events of opening and closing the individual ion channels. Despite this well-known fact, there is a tradition of neglecting the discrete, molecular nature of the bioelectric phenomena. It does not mean there is no space for continuous phenomena: cardiac cells that simultaneously enter and maintain the active state form a wave which travels through space and time. The direct result of this wave, which propagates within the source, is a wave of electric polarization, which travels through the tissue outside the heart. Interestingly, due to the source's frequency range, the velocity of this tissue wave is relatively low: 1500 m/s - substantially slower than the light in a vacuum [1]. Our main result is a mathematical model of the ECG motivated by molecular phenomena. It allows us to investigate the biopotential scene from the perspective of an ECG electrode [2]. Despite its simplicity, the model will enable us to mimic many essential physiological and pathological ECG features.

Concerning the tissue, we treat it as a combination of a dielectric and conductor, which is, however, confined, as the medium has a mesoscopic structure, i.e. the biological cells. The presence of this structure alters the response to physical fields. We denote a surprising lack of the kinetic theory of electrolyte polarization, which would be essential to explain how the electrolyte responds to external charge, which is harmonic in time. This open interdisciplinary problem is essential not only for cardiology, biophysics or biomedical engineering but also for electrochemistry, energy storage and many other industrial contexts, especially those related to the interpretation of Electric Impedance Spectroscopy results [3]. A long-forgotten warning was delivered by nobody else but Cole himself [2] that the equivalent circuit in impedance measurement should not be unequivocally taken for physical reality. Many examples of such misleading systems have been published [4].

There are certain intermediate steps on the way to this kinetic theory: equilibrium theory based on Debye-Hückel equation [5], and the kinetic theory for constant source based on Smoluchowski-Poisson-Boltzmann equation [6]. There exists a broad scope of motivations why this universal mathematical problem is worth tackling.

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APPLICATION OF INFORMATION CONTENT ANALYSIS TO DESCRIPTION OF CARDIOVASCULAR SYSTEM ACTIVITY USING IMPEDANCE CARDIOGRAPHY SIGNALS

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The analysis of cardiovascular system response to various physiological stimuli as for example active orthostatic maneuver, head-up tilt test, handgrip or dynamic exercise may provide some supplementary diagnostic data on autonomic control activity and might help to predict the occurrence of some critical events, e.g. orthostatic syncope. Heart rhythm/rate variability (HRV) has been intensively studied in supine and other body positions in humans. However, only limited study results were published describing rhythms, fluctuations and generally dynamics of hemodynamic parameters, especially monitored during transient phase of physiological tests. Impedance cardiography (ICG) stroke volume and systolic time intervals (STI) changes (including their variability) seems to be a potential source of diagnostic information on mutual coupling between the cardiovascular system and autonomic nervous system dysfunction or modification induced by several environmental and/or pathological factors. Possibly, it could be used for: monitoring the effects of neurodegenerative processes, analysis of sleep apnea disorders, monitoring the effectiveness of physical training and exercise and predicting orthostatic intolerance. Cybulski et al. evaluated short-term variability in hemodynamic parameters - stroke volume (SV), ejection time (ET), pre-ejection period (PEP) –observed in the supine and tilted positions in young women [1] and men [1]. The aim of this study is to deliver the review of some possibilities and prospects of extracting diagnostic information from analysis of impedance cardiography signals (ICG).

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HEART RATE ASYMMETRY IN RELATION TO RESPIRATORY PHASE IN HEALTHY SUBJECTS AND PATIENTS WITH HYPERTATION

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Heart rate asymmetry (HRA) is a physiological phenomenon related to unequal contribution of decelerations and accelerations to heart rate variability (cf. [1] and references therein). We assessed HRA in healthy adults and patients with hypertension. All subjects were examined in supine position and had a regular breathing pattern. We considered 20-minute recordings of ECG and respiration. Each RR interval was assigned to one of four states corresponding to the phase of breathing: inspiration or expiration, and two possible breathing phase transitions: from inspiration to expiration or from expiration to inspiration. Poincaré plots for pairs of RR intervals in subsequent respiratory states for both groups were obtained and described using Guzik's Index, Porta Index and their generalization: Multistructure Index (cf. [2],[3]). We observed that there are significant differences between values of asymmetry indices in dependence of the respiratory state within each considered group and also between respective respiratory states of healthy adults and patients with hypertension.

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RECONSTRUCTING IN-DEPTH ACTIVITY FOR CHAOTIC SPATIO-TEMPORAL EXCITABLE MEDIA MODELS BASED ON SURFACE DATA

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The cardiac muscle is a type of excitable tissue that can exhibit intricate dynamics, including spatio-temporal chaos that is associated with life-threatening cardiac arrhythmias. At a small scale, the cardiac tissue is composed of interconnected cardiac muscle cells that are embedded in an extracellular matrix. These cells interact both electrically and mechanically, and their synchronous or asynchronous movement is triggered by the propagation of electrical excitation waves, which can include spiral or scroll waves during ventricular fibrillation. While it is possible to optically measure electrical excitation on the surface of Langendorff-perfused isolated hearts using fluorescent dyes, methods to reconstruct excitation within the muscle from surface data are required. Two approaches to this reconstruction are presented, a purely data-driven approach, by means of artificial neural networks [1] and a novel approach, called physNODE [2], that combines explicit prior model knowledge, given as ODEs, with continuous adjoint sensitivity analyses related to artificial neural network principles. These approaches are validated on a simple model of isotropic, chaotic excitable media on a regular grid. Our investigations demonstrate that the reconstruction of these high-dimensional chaotic states is theoretically possible, although the quality of the reconstruction depends on various factors and hyperparameters associated with the selected approaches. This contribution presents and discusses the results of these two approaches and compares them with one another.

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OPTOGENETIC CONTROL OF CARDIAC ARRHYTHMIAS

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Rotating spiral waves in the heart are associated with life-threatening cardiac arrhythmias. Today, strong, globally resetting electrical shocks are used to terminate cardiac fibrillation. Significant side effects have motivated the development of alternative low-energy approaches. For this purpose a detailed understanding of the dynamics of spiral waves is required. Cardiac optogenetics opens novel paths to study the mechanisms underlying the onset, perpetuation, and control of cardiac arrhythmias. The termination of ventricular arrhythmias has been demonstrated in optogenetic Langendorff-perfused mouse hearts using global and structured illumination. In this study, we use optogenetics as a tool to numerically and experimentally investigate the control method of resonant feedback pacing, in which global repetitive illumination is applied to cardiac tissue.

We study the control of arrhythmias in N = 5 intact Langendorff-perfused murine hearts expressing ChR2 using two protocols: (i) a single light pulse (SP) (duration 10 and 100 ms, wavelength 470 nm) and (ii) resonant feedback pacing (RFP) with a sequence of global light pulses (duration 20 ms, wavelength 470 nm). The termination success rate is determined as a function of light intensity (LI) for both protocols. Electrocardiogram (ECG) recording and potentiometric optical mapping (dye Di-4-ANBDQPQ) are used to measure cardiac activation before, during, and after optical control. Corresponding numerical simulations of electrical activity of cardiac tissue are performed using the Bondarenko model coupled with a channelrhodopsin-2 model in a 2-dimensional domain 25×25 mm^2. For the RFP method, the dose-response curve shows a termination rate of more than 50% at the lowest LI of 3.1 μW/mm2, while the SP method achieves this rate at a LI two orders of magnitude higher ($\mathrm{LI}_{50}^{SP} = 150$ or 300 μW/mm^2). Moreover, the termination rate at a LI of 100 μW/mm^2 is 100% and 45% for the two control methods of RFP and SP, respectively. Numerical simulations show a dose-response consistent with the experimental findings. At very low LIs, simulations suggest that the underlying mechanism for arrhythmia termination is the spatial shift of the reentry core, termed drift, caused by temporal modulation of cardiac tissue excitability during resonant feedback pacing. Using optogenetics we show that resonant feedback pacing has an exceptional efficiency in terminating arrhythmias in numerical simulations and experimentally in intact mouse hearts.

EVALUATION OF PREDICTIVE ABILITY OF MARKERS ADDED TO RISK PREDICTION MODELS

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Risk prediction models are widely used in many fields of medicine and epidemiology. They enable to identify patients at a high risk of certain adverse effects early and effectively. This can lead to more optimal clinical decisions, better patient prognosis, and improved health of the population in general. One of the most influential epidemiological studies is the Framingham Heart Study, which aims to identify new risk factors of cardiovascular diseases. However, before a new risk factor is added to the current predictive model, its ability to improve the model's prediction needs to be assessed. We propose a new quantitative and graphical method to assess the usefulness of a candidate marker, i.e. the U-smile method, and present it using the Heart Disease Dataset from the UCI Machine Learning Repository.

ON THE PREDICTION OF THE MAXIMAL OXYGEN UPTAKE FROM THE DYNAMIC MODEL

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Maximum oxygen uptake (VO2max) is considered the gold standard in the assessing physical performance. However, its direct measurement in ergospirometric tests is demanding. In athletes, it limits disposition during training process and in the competitions. In patients (especially symptomatic), VO2max determination may be even impossible. What is more, there are restrictive measurement conditions and criteria (unfortunately still inconsistent) for achieving VO2max [1]. For this reason, indirect techniques for estimating VO2max are very popular (models using resting parameters or field tests). The high accuracy of VO2max prediction with an introduction of a protocol that can be used in a wide population is still expected.

We proposed an approach based on a submaximal effort, in which the prediction of VO2max is carried out from dynamic model in form of linear ordinary differential equation [2]. The procedure takes into account the VO2 data and heart rate (HR) monitored during controlled effort. Using retrospective data (from 17 subjects performing an incremental cycling test until exhaustion), we established the moment for effort termination in submaximal trials (80% of maximal HR). We tested the method of prediction on nine young healthy volunteers (five males and four females). The mean relative error of the prediction is 5.56+/-3.92% and is better than results obtained for one of the standard methods in VO2max estimation (Jurca's model), for which this error exceeds 10%. Our prediction should be considered as satisfactory, while it corresponds to the intraindividual day-to-day variation in determination VO2max (between 4% to 6% in healthy subjects and twice higher for patients). The additional strength of the method is reproducing the kinetics of the VO2 response to the exercise, which is not practiced in VO2max estimation but has clinical value [3]. However, the correct transfer of this solution to specific groups of patients requires validation of the prediction accuracy and safety of proposed protocol.

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ENTROPY-BASED METHODS IN THE ANALYSIS OF LONG-TERM ECG RECORDINGS

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The aim of the study was to examine the discriminating capability of various types of entropy measures applied for long-term ECG series. In this research we used five entropy-based methods: Permutation Entropy, Block Entropy, Generalized Permutation Entropy, and two Incremental Permutation Entropies (cf. [1], [2], [3]). Data from two groups of subjects were considered: healthy individuals with normal sinus rhythm and patients with congestive heart failure. We analyzed long-term ECG recordings (of length 75 thous. RR intervals) taken from PhysioNet database [4]. The results confirmed that the entropy-based methods are able to separate the two groups, and thus are promising tools in cardiovascular research as indicators of pathological states.

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MS 08

Organizers: Róbert Horváth

Abstract This minisymposium is dedicated to the investigation of efficient numerical solutions of ordinary and partial differential equations. Of course, the main requirement is the convergence of the methods but the time that is needed to obtain the result or the reliability of the solution is also of high priority in practice. The solution time can be decreased by higher order methods, while the reliability can be achieved by choosing the discretization parameters (the mesh and the time step) appropriately. In the talks of the minisymposium, the construction of higher order methods will be discussed for operator splitting methods applied to ordinary differential equations. The reliability will be guaranteed by giving conditions for the preservation of some qualitative properties of the solutions of ordinary and partial differential equations. We will consider the nonnegativity preservation property, the preservation of some invariants and the validity of maximum minimum principles.

	Monday
Room	CR 113
15:30-15:55	Bálint Takács
15:55-16:20	Lívia Boda
16:20-16:45	István Faragó
16:45-17:10	Róbert Horváth

EFFICIENT NUMERICAL METHODS FOR EPIDEMIC MODELS

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In mathematics there are several problems which can be described by differential equations with a particular, highly complex structure. Most of the time, we cannot produce the exact solution of these problems, therefore we approximate them numerically by using some numerical method. In this talk we analyse some methods, based on operator splitting, which approximate the exact solution of original ODE systems well while having a low computational complexity. The two most popular methods include the sequential splitting (SS) and the Strang–Marchuk (SM) splitting. We analyse the relationship between these methods and at the same time we discuss the properties of processed integrator methods (PIM). Then we generalize these methods and introduce the new extended processed methods (EPM) and the economic extended processed methods (EEPM) with low computational complexity. We test these methods in epidemic models, which play an important role, as these models help in the analysis of the behaviour of diseases. Nowadays, the analysing of these models is becoming more and more important, due to the Covid-19 pandemic in previous years. We solve the SIR model numerically and compare the runtimes and errors.

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SOME QUALITATIVE PROPERTIES OF HTE NONSTANDARD FINITE DIFFERENCE METHOD

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A model of a physical system corresponds to the construction of an approximate mathematical representation of the system, incorporating certain important and essential features of the system, while ignoring everything else [1] Thus, different classes of models are distinguished by which features are reproduced by the model. We consider the dicretization of the Cauchy problem for the ordinary differential equation. Our aim is construct such discrete models which result in convergent numerical solutions, and the discrete solutions preserve the main qualitaive properties of the solution of the continuous model. As it is known, the explicit Runge–Kutta (ERK) methods are insufficient methods for stiff problems, due to lack of A-stability. Moreover, they preserve the nonnegativity only conditionally. These features make them ineffective for dealing with dynamical systems, which are frequently studied over very large time periods. In our talk for the discretization we use the combination of an ERK method with the nonstandard finite difference (NSFD) method [3]. We show that this combined method does not only preserve the consistency order and convergence of the base ERK method but also have many other good features: it is both absolute stable and unconditionally nonnegativity preserving. We demonstrate our theoretical results on the extended Ross model for malaria propagation.

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ON SOME OSCILLATORY PROPERTIES OF FINITE DIFFERENCE METHODS FOR ONE-DIMENSIONAL NONLINEAR PARABOLIC PROBLEMS

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It was shown in [1] that, under some relatively simple conditions, the number of the local maximizers and minimizers of the solution of one-dimensional nonlinear parabolic problems does not grow in time. In this talk we consider the finite difference solutions of the problems and give conditions that guarantee the discrete analogue of the above property. The conditions yield some bounds that restrict the choice of the spatial mesh size and the time step. We use the theory of totally nonnegative matrices [2] in the derivation of the bounds. The results are demonstrated with numerical examples.

Acknowledgments This research was supported by the Hungarian Scientific Research Fund OTKA, No. K137699 and SNN125119.

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POSITIVITY PRESERVING NUMERICAL METHODS FOR EPIDEMIC MODELS

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In recent years the importance of mathematical modeling of propagation of illnesses was highlighted by the outbreak of the Covid-19 epidemic. In this talk we observe an SEIR model (describing the propagation of an illness in a population) with a general incidence rate. Although the qualitative properties of such models were widely studied before (see e.g. [1], [4]), the proper choice for a numerical method which preserves the properties of the original, continuous system remains a crucial problem. In this talk we propose several different methods: strong stability preserving Runge-Kutta methods [3] along with lower and higher order non-standard methods [2], [5]. We give different conditions under which the numerical schemes behave as expected. Then, the theoretical results are demonstrated by some numerical experiments.

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MS 09

Organizers: Manuel Cruz, William Lee, Amélia Caldeira, Matthias Ehrhardt

Abstract EU-MATHS-IN, the European Service Network of Mathematics for Industry and Innovation, is a network of European National Networks representing 20 European countries. The EU-MATHS-IN aims to leverage the impact of mathematics on innovations in key technologies by enhanced communication and information exchange between and among the involved stakeholders on a European level.
This mini-symposium gathers contributions from different EU-MATHS-IN National Networks, presenting success stories of technological transfer between research infrastructures and European industry. These success stories are presented from an industrial perspective and clearly encompass real measurable benefits to the related company, societal challenges, or productive sector.
Moreover, the EU-MATHS-IN OpenDesk, which is a dedicated one-stop shop to coordinate and facilitate the required exchanges in the field of application-driven mathematical research and its exploitation for innovations in industry, science, and society, will be also presented.

	Tuesday
Room	CR 10 D
10:40-11:05	Mauricio Rincón Bonilla
11:05-11:30	Manuel Cruz
11:55-12:20	Valérie Monbet
11:55-12:20	Véronique Maume-Deschamps
15:30-15:55	Anouk Zandbergen
15:55-16:20	Yoann Valero
16:20-16:45	Adérito Araújo
16:45-17:10	Véronique Maume-Deschamps

OPTIMAL CONFIGURATION FOR COMMUNICATION ANTENNA ALONG A RAILWAY LINE

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Solvit is a Portuguese engineering company that develops and implements projects on Information and Communications Technology. On of its main tasks is to provide and maintain stable signal coverage along railway tracks, ensuring quality communications. The company' s challenge for 161st European Study Group with Industry (ESGI), that took place in Portugal last September, is to select, from a number of possible sites, a subset of sites for the installation of antennas in order to ensure stable signal coverage along a railway track, while minimising costs. In this presentation we propose a 0/1 linear optimisation formulation where each selected antenna should try to extend its coverage area while satisfying the company' s requirements regarding coverage area, transmission length and number of antennas.

MODELLING AND SIMULATION OF HYDROGEN DIFFUSION AND EMBRITTLEMENT IN STEELS

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Hydrogen embrittlement (HE) is a phenomenon that causes steels to become brittle and prone to failure. Due to their small size, hydrogen molecules can easily penetrate the steel microstructure and significantly reduce the ductility and load-bearing capacity of the material. Despite great efforts devoted to unraveling the mechanisms behind HE-induced failure and to developing accurate models of processes leading up to it, its multiscale and multimodal nature hinders our ability to fully understand it. At the Basque Center for Applied Mathematics (BCAM) we have partnered with leading research centers and industrial manufacturers in the Basque region of Spain to build a multiscale platform that predicts the effect of processing parameters, microstructure, and composition on the steel response to H adsorption. BCAM is contributing to this platform at the nano and mesoscale levels by investigating the impact of iron vacancies and common steel solutes (such as Mn and Al) on H diffusion in ferritic and austenitic iron. To this end, we employ DFT and free energy methods to estimate the energies associated with H binding and site hopping within a large set of H environments. This information will be used to train an ML based force field that allows us to obtain these energies through classical simulations, greatly reducing the computational burden. Moreover, a surrogate ML model could be subsequently trained to predict unseen energy barriers in a nearly instantaneous fashion. Such a model can be incorporated into a Kinetic Monte Carlo, kMC scheme to simulate H diffusion in realistic structures over large time scales, providing a detailed picture of the H-trapping effect of solutes and vacancies. In addition, the ML force field can be combined with Hamiltonian dynamics (HD) simulations based on our in-house advanced sampling techniques and integrators, thus permitting a direct comparison between kMC and HD and allowing a complete understanding of some of the phenomena leading to HE.

Acknowledgments We acknowledge the financial support by the Ministerio de Economía y Competitividad (MICINN) of the Spanish Government through BCAM Severo Ochoa accreditation CEX2021-001142-S and PID2019-104927GB-C22 grant. This work was supported by the BERC 2022-2025 Program and by ELKARTEK Programme, grants KK-2021/00064, and KK-2022/00006, funded by the Basque Government. The research is partially supported by the Basque Government under the grant Ikerbasque COVID-19. This work has been possible thanks to the computing infrastructure of the i2BASQUE academic network, DIPC Computer Center, RES BSC (QHS-2022-3-0027) and the technical and human support provided by IZO-SGI SGIker of UPV/EHU. We also aknowledge Tecnalia, Tubacex, Glual, Tekniker as our valuable technological and industrial partners.

MEASURING AND FORECASTING THE IMPACT OF THE LIGHT VEHICLE'S ELECTRIFICATION IN THE AUTOMOTIVE MAINTENANCE BUSINESS

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Nors is a Portuguese group whose vision is to be the leader in transport solutions, that sell cars, trucks, buses, machines and construction equipment, parts and service. One of the Nors main challenges in the next few years is to cope with all the disruptions caused by the electrification of light vehicles. Electrification introduces a new set of automotive components and requires new technical skills and capabilities. From the aftermarket point of view, this will imply that some Internal Combustion Engine (ICE) spare parts will become increasingly marginal and ultimately vanish. Moreover, as the Battery Electric Vehicles (BEV) have fewer moving parts they induce less wear which implies lower maintenance costs also impacting the dealers business in the maintenance services. As very few data or publications on this subject are available, is difficult for companies working on the light vehicles business to access the real impact of the transition from ICE to BEV's. LEMA, the Engineering Mathematical Laboratory from Polytechnic of Oporto School of Engineering, has a long-time partnership with the Nors group to provide mathematical technologies to support forecasts and decisions related with the company daily management. In this work, the mathematical model used to forecast the impact of the electrification in the Automotive dealers maintenance services, as well as some preliminary conclusions based on real data will be presented.

ESTIMATION OF MULTIVARIATE GENERALIZED GAMMA CONVOLUTIONS, APPLICATION TO DEPENDENCE STRUCTURE MODELLING IN INSURANCE.

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While modeling the dependence structure between several (re)insurance losses by an additive risk factor model, the infinite divisibility is a very desirable property. Unfortunately, if many useful distributions are infinitely divisible, computing the distributions of their pieces is usually a challenging task that requires heavy numerical computations. We pro- pose an estimation algorithm for multivariate generalized gamma convolutions through Laguerre expansions. These distributions are divisible and useful in dependence structure modeling.

Acknowledgments This work has been partially funded by SCOR SE group. SCOR SE group is now using multivariate gamma convolutions for modelling some of their risk factors in their internal model.

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EU-MATHS-IN OpenDesk. An infrastructure to strengthen the competitiveness of European companies through mathematics

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The European Consortium for Mathematics and Industry (ECMI) and the European Mathematical Society (EMS) launched in 2014 the European Service Network of Mathematics for Industry and Innovation (EU-MATHS-IN) "to leverage the impact of mathematics on innovations in key technologies by enhanced communication and information exchange between and among the involved stakeholders on a European level" (see [1]).

Among other objectives the EU-MATHS-IN Statutes aim: To create a European service unit that can foster the competitive advantage of the European industry through international cooperation.

- To stimulate the cooperation at European level of mathematical research with companies and administrations.
- To establish a one-stop-shop at European level for industrial users of mathematical scientific research results.
- To provide European industry, in particular SMEs, with a competitive advantage taking profit of the scientific excellence of the continent (give Europe the possibility to cash a "scientific dividend").

EU-MATHS-IN was conceived as a network of networks with a single network per country. Nowadays, EU-Maths-IN is present in 20 countries with almost 400 research centres and more than 9,000 researchers specialized in different fields of industrial mathematics. So, EU-MATHS-IN gathers many assets to make companies more competitive through technology transfer between mathematics and industry.

Its vision document [2] published in 2019 analyses the reasons for incorporating mathematics into the productive fabric. On the one hand, the future development of industry and society exhibits strongly increasing complexity and at the same time ever-shorter innovation cycles. On the other hand, digitisation and the internet of things have led to an explosion of data and information. Modelling, Simulation & Optimization in a Data rich Environment (MSO-DE) is the cornerstone for the development of most products in the fields of Industry, Health, Energy or even Finance. Although High Performance Computing, Data Analytics and Artificial Intelligence offer new opportunities, their impact on innovation and the improvement of products and services could remain partial without a massive effort on the axes of modelling, simulation, complex systems optimization, stochastic and statistical learning. Major opportunities, in particular, the establishment of digital twins, rely on the connections at the interface between fields of expertise, domains, businesses and across the complete lifecycle of products & systems. At the same time, methods have outpaced computational power in terms of capability over the past decades. EU-MATHS-IN initiative is guided by the certainty that a high-level approach on Modelling, Simulation & Optimization, enriched by data analytics and intensive computing, is a considerable economic asset.

EU-MATHS-IN vision is also in good agreement with the Age of Mathematics report [3], which concludes that the digital society is deeply dependent on mathematics and algorithms. An idea of the importance that the incorporation of this great potential of mathematics can have for industry is provided by several studies showing the impact of mathematics on the Gross Value Added (GVA) for different countries [4,5,6,7].

After analysing the potential of MSO-DE technology, the strengths and weaknesses of the current network structure, EU-MATHS-IN decided in 2022 to give a new impulse, based on its statutes, launching its OpenDesk ([8], https://opendesk.eu-maths-in.eu/). The EU-MATHS-IN OpenDesk is a one-stop-shop aimed at boosting industrial competitiveness, providing state-of-the-art solutions to innovation projects for industries from all sectors, SMEs, start-ups, and administrations. Ensuring at the same time

transparency, privacy, and confidentiality, OpenDesk facilitates the access of European industry to the best European technology transfer centres existing in Industrial Mathematics, and coordinates the looking for the most appropriate partners to effectively solve their current challenges.

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MIR & STATISTIC MODELING FOR PREDICTION OF NASH DISEASE

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In this paper, a suitable and interpretable diagnosis statistical model is proposed to predict the Non-Alcoholic Steatohepatitis (NASH) [1] from near infrared spectrometry data. In this disease, unknown patients profiles are expected to lead to different diagnosis. The model has then to take into account the heterogeneity of the data and the dimension of the spectrometric data. To this end, we propose to fit a mixture on the joint distribution of the diagnosis binary variable and the covariates selected in the spectra. Because of the high dimension of the data, a penalized maximum likelihood estimator is considered. In practice, a twofold penalty on both regression coefficients and covariance parameters is imposed. Automatic selection criteria such as the AIC and BIC are used to select the amount of shrinkage and the number of clusters. Performance of the overall procedure is evaluated through a simulation study and its application on the NASH data set is analysed. The model leads to higher prediction performance than competitive methods and provides highly interpretable results [2].

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USE OF PROCESS CROWDING IN CONDITIONAL WGAN FOR REMAINING PROCESS EVENTS PREDICTION

Yoann Valero[a,b], **Frédéric Bertrand**[a] and **Myriam Maumy**[a]

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Predictive business process monitoring (PBPM) aims at predicting the future of running units in a process (prefixes), be it for the next event or the remaining sequence of events (suffix), an event being characterized at least by a triplet made of a unit identifier, an activity the unit can go through, and the time of activity execution. For suffix predictions, encoder-decoder generative adversarial networks (GAN) have proven to be most efficient [1]. We improved the model further by using the Wasserstein loss (WGAN) [2] to stabilize and ease its training phase. Our main contribution, however, comes with feature engineering: external, unobserved elements often have an impact on the progress of a process instance, and covariables are hardly ever taken into account in current models, or outright unavailable. We therefore propose a feature engineering method to extract what we call process crowding data, and predict suffixes conditionally to such variables by turning the model into a conditional WGAN [3].We will then show its efficiency at proposing noticeably improved predictions. The creation of process crowding is a breakthrough as it constitutes variables which are loaded with information, easy to extract, and always available in any event log. Process crowding allows for a multitude of uses, one of which is process predictions. The increase in accuracy in predictive models is tremendous, at almost no cost in computation time, training time or memory usage. In turn, Your Data Consulting, now QAD Process Intelligence, is able, through their software Livejourney, to predict process units with accuracy above current state of the art. It allows their customers to not only track and analyze their units in real time, but to also track and analyze the future of ongoing units (and thus their entire processes) with unprecedented accuracy.

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IMPROVING THE CONVERGENCE OF PSEUDO-TRANSIENT CONTINUATION FOR CFD SIMULATIONS USING NEURAL NETWORKS

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Computational fluid dynamics (CFD) simulations are highly relevant for a large range of applications, including but not restricted to the fields of aerospace, environmental, and biological engineering as well as weather predictions and medicine. Modeling Newtonian fluids involves the solution of the Navier-Stokes equations, which, depending on the Reynolds number of the flow, may exhibit a highly nonlinear behavior. Discretization of the PDE yields a nonlinear system of equations, which can be solved using nonlinear iteration methods, such as Newton' s method. However, fast quadratic convergence is typically only obtained in a local neighborhood of the solution, and in many configurations, the classical Newton iteration does not converge at all. In such cases, so-called globalization techniques may help to improve convergence.
In this talk, pseudo-transient continuation as a globalization technique for the stationary Navier- Stokes equations will be considered, and a neural network model will be employed to improve the convergence of Newton' s method. In order to facilitate generalizability of the model, local input and output features are used. In particular, the input features are based on geometrical information as well as the solution and residual vectors on the element level, and the output feature is a local quantity appearing in the pseudo-transient continuation approach, that is, the local CFL (Courant–Friedrichs–Lewy) number.
Numerical results for standard benchmark problems, including flow through a backward facing step (BFS) geometry and Couette flow, are presented to show the performance of the machine learning-enhanced globalization technique; as the software for the simulations, we employ the CFD module of COMSOL Multiphysics

MS 10

Organizers: Karolina Kropielnicka, Łukasz Płociniczak

Abstract The purpose of this minisymposium will be to gather researchers from numerical methods for partial differential equations working both in analysis and applications. Ranging from local to nonlocal, linear to nonlinear, steady to highly oscillatory, the themes of the presented talks will span a broad range of various topics important for modern science and technology.

	Tuesday
Room	CR 115
10:40-11:05	Jan ten Thije Boonkkamp
11:05-11:30	Juan del Valle
11:30-11:55	Karolina Lademann
11:55-12:20	Karolina Kropielnicka
15:30-15:55	Felix del Teso
15:55-16:20	Mateusz Świtała
16:20-16:45	Maria Lopez-Fernandez
16:45-17:10	Łukasz Płociniczak

DG METHODS FOR LIOUVILLE'S EQUATION OF GEOMETRICAL OPTICS

Jan ten Thije Boonkkamp[a], **Robert van Gestel**[a], **Martijn Anthonissen**[a] and **Wilbert IJzerman**[a,b]

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The standard optical systems simulation method is ray tracing. Given an optical system and a source light distribution, we compute the path of a large collection of rays through the system, from source to target. From the distribution of rays at the target we can reconstruct the target distribution. Ray tracing can therefore be interpreted as a Lagrangian method. Recently, we have developed an alternative Eulerian method based on Liouville's equation of geometrical optics [1].

Propagation of light rays can be described by a Hamiltonian system in phase space, i.e., the space of position and direction coordinates of light rays. Combining the Hamiltonian system with conservation of basic luminance, we can derive Liouville's equation, which is a linear advection equation for the basic luminance. For such an equation, there are many numerical schemes available. Propagation of the basic luminance in phase space is rather straightforward, except for optical surfaces (reflector/lens). At an optical interface conservation of basic luminance still holds, however, the direction of a light ray changes discontinuously according to Snell's law or the law of specular reflection, leading to a nonlocal interface condition in phase space.

We have developed several numerical schemes for Liouville's equation [1],[2], in particular discontinuous Galerkin spectral element methods. Our schemes have the following features: high-order spatial discretization, energy conservation and a moving mesh with grid refinement. In addition, our schemes include an energy conservative discretization of the interface condition. For time integration we employ sophisticated schemes, like explicit high-order Runge-Kutta methods and ADER schemes.

We have applied our schemes to several optical systems, and compared these to classical ray tracing. From this we conclude that DG schemes clearly outperform ray tracing.

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ASYMPTOTIC EXPANSIONS FOR THE LINEAR PDEs WITH OSCILLATORY INPUT TERMS: ANALYTICAL FORM AND ERROR ANALYSIS

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Partial differential equations with highly oscillatory input term are hardly ever solvable analytically and they are difficult to treat numerically. Modulated Fourier expansion used as an ansatz is a well known and extensively investigated tool in asymptotic numerical approach for this kind of problems.

In this talk I will consider input term with single frequency and will show that the ansatz need not be assumed –it can be derived naturally while developing formulas for expansion coefficients. Moreover I will present the formula describing the error term and its estimates. Theoretical investigations will be illustrated by results of the computational simulations.

UNIFORM IN OSCILLATIONS NUMERICAL METHODS FOR HIGHLY OSCILLATORY KLEIN–GORDON EQUATION

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High oscillation is a phenomenon occurring in a very wide range of problems in science and engineering and it represents an enduring computational challenge. The main reason is that classical numerical analysis rests upon the concept of truncated Taylor expansion with a small error constant, but this need not be true once high oscillation is present.

An example of equation, where high oscillations play an important role, is the Klein–Gordon equation

$$\partial_t^2 \psi(\mathbf{x}, t) = \Delta \psi(\mathbf{x}, t) + f(\mathbf{x}, t)\psi(\mathbf{x}, t),$$

where input term $f(\mathbf{x}, t)$ is a given function under the form

$$f(\mathbf{x}, t) = \alpha(\mathbf{x}, t) + \sum_{|n| \leq N} a_n(\mathbf{x}, t) e^{i\omega_n t}.$$

I will present several numerical approaches specialized to highly oscillatory input term. The discussed methods show high accuracy and low computational cost. I will briefly discuss the derivation of the methods, error analysis and present plenty of numerical examples comparing derived methods against each other and against other methods known from the literature.

Acknowledgments The authors are grateful for the support of the National Science Centre (NCN), project no. 2019/34/E/ST1/00390.

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GENERALIZED CONVOLUTION QUADRATURE FOR THE FRACTIONAL INTEGRAL AND FRACTIONAL DIFFUSION EQUATIONS

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We consider the application of the generalized Convolution Quadrature (gCQ) of the first order to approximate fractional integrals and associated fractional diffusion equations. The gCQ is a generalization of Lubich's Convolution Quadrature (CQ) which allows for variable steps. In this paper we analyze the application of the gCQ to fractional integrals, with a focus on the low regularity case. It is well known that in this situation the original CQ presents an order reduction close to the singularity. The available theory for the gCQ does not cover this situation. Here we use a different expression for the numerical approximation and the associated error, which allows us to significantly relax the regularity requirements for the application of the gCQ method. In particular we are able to eliminate the a priori regularization step required in the original derivation of the gCQ. We show first order of convergence for a general time mesh under much weaker regularity requirements than previous results in the literature. We also prove that uniform first order convergence is achievable for a graded time mesh, which is appropriately refined close to the singularity, according to the order of the fractional integral and the regularity of the data. Then we study how to obtain full order of convergence for the application to linear fractional diffusion equations. An important advantage of the gCQ method is that it allows for a fast and memory reduced implementation. We outline how this algorithm can be implemented and illustrate our theoretical results with several numerical experiments.

Acknowledgments The speaker is grateful for the support of the "Beca Leonardo for Researchers and Cultural Creators 2022", granted by the BBVA Foundation.

NUMERICAL METHODS FOR THE TIME-FRACTIONAL POROUS MEDIUM EQUATION

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We present some of our results concerning numerical discretizations of nonlinear and fractional in time parabolic equations. Along with a collection of various methods and statements about their convergence and stability, we stress their motivation and real-world applications. The main equation of our concern is the following parabolic PDE

$$\partial_t^\alpha u = \nabla \cdot (D(u)\nabla u), \quad 0 < \alpha < 1,$$

where ∂_t^α is the *Caputo fractional derivative* modeling nonlocal in time phenomena. In this talk we will present several efficient and fast numerical methods for solving the above. Presented results have been published in [1,2,3,4,5].

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ERROR ANALYSIS OF NUMERICAL SCHEME FOR THE ERDÉLYI–KOBER FRACTIONAL DIFFUSION EQUATION

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The aim of this talk is to introduce the numerical scheme for the Erdélyi–Kober fractional diffusion equation. The solution of the considered nonlocal PDE can be thought as the marginal *pdf* of the stochastic process called the *generalized grey Brownian motion* (ggBm). Detailed numerical analysis of the governing PDE is important due to the fact that ggBm includes some well-known stochastic processes: Brownian motion, fractional Brownian motion, and grey Brownian motion. To obtain a convergent numerical scheme for the Erdélyi–Kober fractional diffusion equation, we transform the analysed equation into its weak form and apply the appropriate discretization of the Erdélyi–Kober fractional derivative. During my talk, I am going to propose two discretization methods for the Erdélyi–Kober fractional derivative, together with the presentation of the estimates on the discretization errors [1]. The analysis includes also the case when the derivatives of the function upon which the Erdélyi–Kober fractional operator acts, have a power-type singularity at the initial point.

In further analysis of the main fractional equation, we prove the stability of the solution of the semi-discrete problem and its convergence to the exact solution [1]. Furthermore, the numerical and analytical studies of the full-discrete problem will be presented, where orthogonal expansion in terms of the Hermite functions with respect to the spatial dimension is used. Due to the singular behaviour of the exact solution with respect to time variable, the proposed method converges slower than first order.

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A CONVERGENT DISCRETIZATION OF THE POROUS MEDIUM EQUATION WITH FRACTIONAL PRESSURE

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We carefully construct and prove convergence of a numerical discretization of the porous medium equation with fractional pressure,

$$\frac{\partial u}{\partial t} - \nabla \cdot \left(u^{m-1} \nabla (-\Delta)^{-\sigma} u \right) = 0, \tag{FPE}$$

for $\sigma \in (0,1)$ and $m \geq 2$. The model, introduced by Caffarelli and Vázquez in 2011, is currently one of two main nonlocal extensions of the local porous medium equation. It has finite speed of propagation, but as opposed to the other extension, it does not satisfy the comparison principle. We exploit the fact that the *cumulative density* $v(x,t) = \int_{-\infty}^{y} u(y,t)dy$ satisfies

$$\frac{\partial v}{\partial t} + |\partial_x v|^{m-1} (-\Delta)^s v = 0, \quad s = 1 - \sigma,$$

which is a nonlocal quasilinear parabolic equation in non-divergence form that can be analyzed through viscosity solution methods.

The numerical method consists in discretizing this equation with a difference quadrature scheme with upwinding ideas and then compute the solution u of (FPE) via numerical differentiation. Our results cover both absolutely continuous and Dirac or point mass initial data, and in the latter case, machinery for discontinuous viscosity solutions are needed in the analysis.

This is a joint work with E. R. Jakobsen.

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A NEW PICTURE ON THE STRANG SPLITTING

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Strang splitting is a well-established and widely used technique for finding approximate solutions of linear differential equations of the type $u' = (A + B)u$, where A and B are time-independent components. However, it can also be used for the case of time-dependent component $B(t)$ after the application of the mid-point quadrature rule at the level of the Magnus expansion.

In this talk, I will show how Strang splitting scheme for time-dependent components can be derived using the Duhamel formula. Based on this approach, I will (i) present a new proof of convergence of this second order scheme and (ii) elaborate on the possibilities brought by this approach concerning higher order methods. A concrete analysis of the error estimated and numerical simulations will be presented for the physically relevant example of a hydrogen atom featuring the singular Coulomb potential.

MS 11

Organizers: Imre Fekete, Ferenc Izsák

Abstract As a powerful tool in computational mathematics, artificial neural networks can contribute to the numerical solution of ODEs and PDEs. Furthermore, using neural ODE' s, existing solvers can enhance the efficiency of certain neural networks. A family of artificial neural networks can offer completely new numerical solutions (e.g., in the framework of physics-informed neural networks), while another family of them can enhance the efficiency of existing conventional PDE and ODE solvers.
Within this minisymposium, related results are presented supporting the collaboration in this wide research field.

	Monday
Room	CR 115
10:40-11:00	Davide Murari
11:00-11:20	Giulia Bertaglia
11:20-11:40	Karl Schrader
11:40:12:00	Tatiana Kossaczká
12:00-12:20	András Molnár

SOLVING MULTISCALE PROBLEMS WITH NEURAL NETWORKS: THE IMPORTANCE OF ASYMPTOTIC–PRESERVATION

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Data-driven approaches have begun to gain popularity throughout science, leading to a fundamental change in the scientific method as a result of the rapid advancement of Machine Learning techniques and the enormous increase in the availability of scientific data. However, the use of conventional Deep Neural Networks (DNNs) or even conventional Physics-Informed Neural Networks (PINNs) to analyse the dynamics of complex multiscale systems can lead to incorrect inferences and predictions. This is due to the presence of small scales leading to simplified or reduced models in the system that must be satisfied during the learning process. In this talk, these problems will be addressed in light of recent results obtained in the development of Asymptotic-Preserving Neural Networks (APNNs) for hyperbolic models with diffusive scaling [1,2]. A series of numerical tests will demonstrate how APNNs significantly outperform traditional DNNs and PINNs at various model scales, particularly when examining cases where only sparse information is available.

Acknowledgments The author acknowledges the support by INdAM-GNCS.

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DISCRETIZATION ERRORS IN FINITE DIFFERENCE SCHEMES APPROXIMATED BY DEEP LEARNING

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We present our approach to enhance finite difference schemes by deep learning. To achieve this aim, we utilize a convolutional neural network to approximate the local truncation error of standard finite difference schemes. Using this technique, we preserve the convergence and consistency properties of the original method and achieve higher numerical accuracy in presented examples. We introduce our scheme as a proof of concept, which aims to enhance the standard and compact finite difference methods, but it can be easily adapted to enhance other numerical methods as well [1].

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A FUNCTIONAL APPROACH TO INTERPRETING THE ROLE OF THE ADJOINT EQUATION IN MACHINE LEARNING

Imre Fekete[a,b], **András Molnár**[a] and **Péter L. Simon**[a,b]

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The connection between differential equations and machine learning has recently been revealed. A key issue shared by both fields is the inverse problem of fitting parameters to minimize the difference between data and model output. Our paper [1] explores an abstraction that can be used to construct a family of loss functions with the aim of fitting the solution of an initial value problem to a set of discrete or continuous measurements. We show that an extension of the adjoint equation can be used to derive the gradient of the loss function as a continuous analogue of backpropagation in machine learning. Numerical evidence is presented that under reasonably controlled circumstances, the gradients obtained this way can be used in a gradient descent to fit the solution of an initial value problem to a set of continuous noisy measurements, and then to a set of discrete noisy measurements that are recorded at uncertain times.

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LEARNING HAMILTONIANS OF CONSTRAINED MECHANICAL SYSTEMS

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Recently, there has been an increasing interest in the modelling and computation of physical systems with neural networks. Hamiltonian systems are an elegant and compact formalism in classical mechanics, where the dynamics is entirely determined by one scalar function, the Hamiltonian. The solution trajectories of Hamiltonian systems are often constrained to evolve on a submanifold of a linear vector space. Thus, after a brief overview of the unconstrained case, we derive a strategy to approximate constrained Hamiltonian vector fields with neural networks. In particular, we show how numerical methods are involved in this approximation task, focusing on the importance of preserving the constrained space of the system during the learning procedure. This talk is based on the paper [1].

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TRANSLATING ANISOTROPIC DIFFUSION INTO RESIDUAL NETWORKS

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Anisotropic diffusion filtering with a matrix-valued diffusion tensor [3] is an established technique for image denoising and inpainting-based image compression. While processes with strong anisotropy can produce good results, designing high-quality discretisation for them is non-trivial.

We introduce the δ-stencil class that subsumes many spatial finite difference discretisations. It can be derived by splitting the 2-D diffusion process into four 1-D diffusions. It is an equivalent but simpler representation of the stencil family from [4] that involves two parameters and offers state-of-the-art performance in terms of rotation invariance and low dissipativity.

Furthermore, we present a direct translation of an explicit scheme based on the δ-stencil into a neural architecture. For suitable weights and activation functions, a ResNet block [2] performs one iteration of an explicit scheme. This translation extends recent results by Alt et al. [1] from the isotropic to the anisotropic setting. We derive this result from the directional splitting decomposition of the stencil. This allows a direct implementation of anisotropic diffusion in deep learning architectures. The resulting highly efficient GPU implementations are straightforward and require no time-consuming optimisation of low-level CUDA code.

Furthermore, we perform a detailed stability analysis of the δ-stencil in the Euclidean norm. It aims at large time step size bounds that take into account the stencil parameters as well as the eigenstructure of the diffusion tensor.

These advances allow for more efficient implementations of anisotropic diffusion and its integration into neuroexplicit methods in our ongoing work.

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MS 12

Organizers: Matthias Ehrhardt, Björn Liljegren-Sailer

Abstract The minisymposium focuses on the port-Hamiltonian approach for modelling and analysing complex dynamic systems. This approach is strongly related to the notions of passivity, port-based modelling and Dirac structures. Topics to be discussed include, but are not limited to:

- Computational causality
- Hierarchical modelling
- Infinite-dimensional systems
- Well-posedness
- Control of finite-dimensional systems
- Numerical methods
- Model reduction
- Discrete-time systems
- Stochastic systems

	Monday
Room	CR 114
11:30-12:20	Chairperson: B. Liljegren-Sailer
10:40-11:05	Hannes Gernandt
11:05-11:30	Malak Diab
11:55-12:20	Andrea Brugnoli
11:55-12:20	Sølve Eidnes
15:30-17:10	Chairperson: M. Ehrhardt
15:30-15:55	Michael Günther
15:55-16:20	Björn Liljegren-Sailer
16:20-16:45	Sarah Hauschild
16:45-17:10	Philipp Schulze
17:20-18:35	Chairperson: B. Liljegren-Sailer
17:20-17:45	Najmeh Javanmardi
17:45-18:10	Markus Lohmayer
18:10-18:35	Nathanael Skrepek

HYBRID FINITE ELEMENTS FOR PORT-HAMILTONIAN SYSTEMS

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Numerical methods to discretize port-Hamiltonian systems need to retain their geometric structure in order to be successfully used for complex multiphysical applications. In this talk, a continuous Galerkin finite element exterior calculus formulation that is able to mimetically represent coupled conservation laws and their power balance is presented. The possibility of including open boundary conditions allows for modular composition of complex multi-physical systems whereas the exterior calculus formulation provides a coordinate-free treatment. The power balance characterizing the Stokes-Dirac structure is retrieved at the discrete level using the de Rham complex properties and symplectic Runge-Kutta integrators based on Gauss-Legendre collocation points. The proposed formulation is directly amenable to hybridization. The hybrid formulation is equivalent to the continuous Galerkin formulation and can be efficiently solved using a static condensation procedure in discrete time, leading to a much smaller system to be solved.

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OPERATOR SPLITTING FOR SEMI-EXPLICIT DAEs AND PHDAEs

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Operator splitting methods allow to split the operator describing a complex dynamical system into a sequence of simpler sub-systems and treat each part independently. In the modeling of dynamical problems, systems of (possibly coupled) differential-algebraic equations (DAEs) arise. This motivates the application of operator splittings which are aware of the various structural forms of DAEs. Here, we present an approach for the splitting of coupled index-1 DAE as well as for the splitting of port-Hamiltonian DAEs, taking advantage of the energy-conservative and energy-dissipative parts. We provide numerical examples illustrating our second-order convergence results.

MACHINE LEARNING OF PSEUDO-HAMILTONIAN SYSTEMS

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Recent advancements in machine learning models utilizing Hamiltonian formulations have shown promising results for both energy-conserving and non-energy-conserving simple mechanical systems. In [1], we presented the pseudo-Hamiltonian formulation, a slight generalization of the port-Hamiltonian formulation, which again generalizes the Hamiltonian formulation. We illustrated how neural network models incorporating a pseudo-Hamiltonian structure can effectively learn external forces impacting a system. This feature is particularly advantageous when external forces depend on the state, in which case the pseudo-Hamiltonian structure is utilized to distinguish between internal and external forces. In this presentation, we will showcase findings from our previous work [1] and new results that demonstrate the potential advantages of integrating pseudo- or port-Hamiltonian structures in neural network models.

Furthermore, we will explore the application of pseudo-Hamiltonian formulations to machine learning models beyond neural networks, particularly focusing on pseudo-Hamiltonian system identification. Identifying the accurate differential equations that govern a system using only observational samples can be a challenging task. By assuming a specific pseudo-Hamiltonian structure for the system under investigation, we can determine the analytic terms of internal dynamics, even when the model is trained on data influenced by unknown damping and external disturbances. In situations where determining analytic terms for the disturbances is difficult, a hybrid model that uses a neural network to learn these disturbances can still accurately identify the system's dynamics as if under ideal conditions. This approach renders the models viable in scenarios where traditional system identification models fall short.

Acknowledgments The research was supported by the Research Council of Norway through the projects BigDataMine (no. 309691) and TAPI: Towards Autonomy in Process Industries (no. 294544).

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ON DISCRETE-TIME PORT-HAMILTONIAN (DESCRIPTOR) SYSTEMS

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In this talk, we develop a discrete-time port-Hamiltonian (pH) formulation for linear dynamical systems that is purely based on the system coefficients. First, we recall pH continuous-time (descriptor) systems and study the their relation to passive and positive real systems [1]. Based on this, the definition of scattering passive pH (descriptor) systems from [2] is given. Furthermore, we study the relation to positive and bounded real systems and existence of positive semidefinite solutions of Kalman-Yakubovich-Popv inequalities.

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OPERATOR SPLITTING FOR PORT-HAMILTONIAN ORDINARY DIFFERENTIAL EQUATIONS: EFFICIENT LINEAR EQUATION SOLVERS AND MULTIRATE TECHNIQUES

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The port-Hamiltonian approach presents an energy-based modeling of dynamical systems with energy-conservative and energy-dissipative parts as well as an interconnection over the so-called ports. In this paper, we apply an operator splitting that treats the energy-conservative and energy-dissipative parts separately. This paves the way for linear equation solvers to exploit the respective special structures of the iteration matrices as well as the multirate potential in the different right-hand sides. We illustrate the approach using test examples from coupled multibody system dyn

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STRUCTURE-PRESERVING METHODS FOR COUPLED pH-SYSTEMS OF NON-ISOTHERMAL FLUID FLOW

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The port-Hamiltonian formulation of partial-differential equations and their numerical treatment have been elaborately studied lately. One advantage of port-Hamiltonian systems is that fundamental physical properties, like energy dissipation and mass conservation, are encoded in the system structure. Therefore, structure-preservation is most important during all stages of approximation and system coupling. In this context we consider the non-isothermal flow of a compressible fluid through a network of pipes. Based on a port-Hamiltonian formulation of Euler-type equations on one pipe [1], we introduce coupling conditions, through which we can realize energy, mass and entropy conservation at the coupling nodes and thus, preserve the port-Hamiltonian structure. We implement them through an input-output-coupling using the flow and effort variables of the boundary port of the underlying Dirac structure. Thus, we can make use of the structure-preserving model and complexity reduction techniques for the single pipe [2]. This procedure becomes even more important for network simulations, as here, we deal with high dimensional and highly non-linear dynamical systems. We explain the extension from a single pipe to a network and numerical examples are shown to support our findings.

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ENERGY-BASED CONTROL APPROACHES FOR ELECTROMECHANICAL SYSTEMS

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Electromechanical (EM) systems have been utilized in a wide range of industrial applications, such as electric drives, robotics, and micro/nanoelectromechanical systems (MEMS/NEMS). EM systems consist of the interconnection of mechanical and electrical subsystems. Customarily, the coupling between these subsystems is captured by nonlinear functions in the energy of the EM system. In particular, these highly nonlinear couplings may lead to a saddle-node bifurcation phenomenon called pull-in instability, which is one of the critical practical issues in weakly coupled EM systems, e.g., MEMS devices [2]. As a result, the performance and operation range in weakly coupled EM systems are significantly limited by the inherent instability of these systems. In this talk, we will discuss the following control challenges:

- How to stabilize weakly coupled EM systems via static controllers, such that the trajectories of the closed-loop system converge to an assignable desired equilibrium?
- How to solve the trajectory-tracking problem for weakly coupled EM systems?

To this end, we use the port-Hamiltonian (pH) framework, which offers a unified and systematic framework for modeling and control EM systems. Then, we propose control methods based on the concepts of energy shaping [4] and contractive systems [3]. The resulting controllers have physical interpretation, do not require solving partial differential matching equations and implementing any change of coordinates. Besides, we will discuss other topics, such as the exponential stability of the desired equilibrium/trajectory and the performance of the closed-loop system.

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SNAPSHOT-BASED MODEL REDUCTION FOR PORT-HAMILTONIAN SYSTEMS

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The port-Hamiltonian framework can be used for the structured modeling of dynamical systems, cf. [1]. Its modularized nature and energy-based interpretation have shown to be advantageous for the design of structured approximations as well. In this talk, we are concerned in the efficient, structure-preserving approximation of large-dimensional nonlinear systems with model reduction techniques. More specifically, an adapted variant of the snapshot-based model order reduction method Proper Orthogonal Decomposition is combined with quadrature-based complexity reduction. The method has been developed in [2] for the approximation in space. An adaption to the approximation in time, cf. [3], is currently under investigation.

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EXERGETIC PORT-HAMILTONIAN SYSTEMS

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Mathematical modeling of real-world physical systems requires the consistent combination of many different physical laws and phenomenological models. Modular and hierarchical decomposition of systems can greatly simplify the modeling process and enable reuse of parts of the model. A graphical expression of the decomposition of a complex model into its ultimately simple parts gives structure to the modeling process and facilitates communication. As an important requirement, models and their parts are expected to satisfy the laws of thermodynamics as well as other fundamental conservation laws. While some modeling frameworks exist which guarantee fundamental physical laws based on structural properties of their models, they do not have a graphical syntax to express the modular and hierarchical decomposition of their models into primitive components. We present results on the mathematical formalization of a compositional and thermodynamically consistent modeling language with a graphical syntax. Our approach endows port-Hamiltonian systems with further structural properties and a fixed physical interpretation such that thermodynamic consistency is ensured in a way that is closely related to the GENERIC framework for nonequilibrium thermodynamics. Port-Hamiltonian systems have a close connection to the graphical modeling approach termed bond graphs but neither bond graphs, nor the connection can be easily formalized. In contrast, the syntax of our language forms a category where composition expresses the hierarchical nesting of subsystems. The language effectively decouples the physical concerns of modeling which only need to be dealt with at the level of primitive subsystems from the compositional concerns which are handled by its syntax. Due to the taken exergetic perspective on nonequilibrium thermodynamics, the language seems particularly well suited for analysis and optimization of thermodynamic systems.

NONLINEAR MODEL REDUCTION FOR TRANSPORT-DOMINATED PORT-HAMILTONIAN SYSTEMS

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Classical model order reduction (MOR) methods are usually based on projecting the full-order model (FOM) onto a suitable low-dimensional linear subspace. However, such linear approaches are often ineffective when applied to systems whose dynamics are dominated by the propagation of waves with sharp fronts. This is one of the reasons why MOR techniques based on nonlinear approximation ansatzes have received more and more attention in the past years.

In this talk, we demonstrate how to achieve structure-preserving model reduction for port-Hamiltonian systems based on a special class of nonlinear approximation ansatzes, cf. [1]. In particular, we consider separable ansatzes which are characterized by the fact that they are linear with respect to a part of the reduced-order model (ROM) state variables. Such approaches are especially relevant in the context of transport-dominated systems, for instance, when the FOM state is approximated by a linear combination of dynamically transformed modes, cf. [2]. We show that a port-Hamiltonian ROM may be constructed in an optimal way by minimizing the residual in a suitably weighted norm. As a consequence, one may also show stability of the ROM in the sense that the resulting approximation of the FOM state remains bounded over time. Furthermore, we illustrate that using a time discretization scheme based on a modified discrete gradient approach leads to a power balance on the time-discrete level. Finally, the new approach is illustrated by means of a numerical example.

Acknowledgments The author is grateful for the support of the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) Collaborative Research Center Transregio 96 *Thermo-energetic design of machine tools – A systemic approach to solve the conflict between power efficiency, accuracy and productivity demonstrated at the example of machining production*, project number 174223256.

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A PORT-HAMILTONIAN APPROACH TO COUPLED CABLE-FIELD PROBLEMS

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We investigate the electromagnetic interactions of cable harnesses. We model every single cable as a 1-D transmission line, which is embedded in a 3-D electromagnetic field. The cables interact with each other via this 3-D field, which is modeled by Maxwell's equations. Hence, every single component of our model fits into the framework of port-Hamiltonian systems. However, the difficulty that arises in the coupling is the mismatch of dimensions. We will overcome this issue by a similar approach as in [1]. This is by lifting the dynamics of the 1-D transmission line on a 2-D surface, which fits the boundary ports of Maxwell's equations. Moreover, we go beyond the description of the model as in [1] and show well-posedness of the coupled system.

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MS 13

Organizers: Alessandra Micheletti, Natasa Krejic

Abstract The availability of huge amounts of data is often considered as the fourth industrial revolution we are living right now. The increase in data accumulation allows us to tackle a wide range of social, economic, industrial and scientific challenges. But extracting meaningful knowledge from the available data is not a trivial task and represents a severe challenge for data analysts.
Mathematics is the 'language' on which are based the existing algorithms for data processing and for AI. This minisymposium is organized within the ECMI SIG "Mathematics for Big Data and AI" . The talks in this minisymposium will present and discuss how Mathematics can play a leading role in improving the reliability, computational efficiency, and transparency of the existing techniques for big data analysis and AI.

	Tuesday
Room	CR 10 D
17:20-17:45	Lidija Fodor
17:45-18:10	Alessandra Micheletti
18:10-18:35	Diogo Lavado
18:35-19:00	Claudia Soares

A DISTRIBUTED INEXACT LEVENBERQ MARQUARTD METHOD FOR NONLINEAR LEAST SQUARES

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We propose an inexact Levenberg Marquardt method for nonlinear least squares problems of very large dimension. The method is suitable for master/workers distributed computational framework. At each iteration of the proposed method, a search direction is computed by approximately solving the linear Levenberg Marquardt system in distributed manner, using a fixed point strategy that relies on the partition of the variables induced by the near-separability property. The master node aggregates the local solutions and then perfoms a nonmonotone line search in each iteration. We prove that the method converges globally, while the local convergence order depends on the choice of the parameters of the method. Aside from near-separability, the required assumptions are the same as for the convergence analysis of classical Levenberg Marquardt method. Numerical results that confirm theoretical analysis are also presented.

SCENE-NET: LEVERAGING GROUP EQUIVARIANCE FOR GEOMETRIC INTERPRETABILITY IN MACHINE LEARNING

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Machine learning poses a crucial challenge in developing models that are both accurate and trustworthy while being scalable to large datasets. This challenge is particularly pertinent given the wide application of machine learning methods to high-risk domains such as autonomous driving, where the reliability of models are of utmost importance. In this work, we take advantage of group equivariant non-expansive operators (GENEOs) [1] as a powerful tool for achieving geometric interpretability in machine learning. GENEOs are operators that observe topological spaces, such as point clouds, and are designed to respect certain symmetries in the data while transforming it. In other words, they transform data into higher-level representations while respecting a predefined set of meaningful features, making them particularly suitable for data analysis and feature extraction. We propose a novel white-box model, SCENE-Net, that leverages on GENEOs to provide intrinsic geometric interpretability. SCENE-Net identifies signature shapes in point clouds by transforming them into high-level spaces, where it is easier to distinguish between different objects. We applied our model to a challenging real-world problem, namely the detection of power line supporting towers, to reduce human effort in inspecting large power lines—a key task in the prevention of forest fires and large-scale power outages. SCENE-Net offers robustness to noisy data and low-resource deployment and has on-par performance with state-of-the-art methods.

Our work showcases the potential of GENEOs as a mathematical framework for developing trustworthy and interpretable machine learning. By exploiting equivariance, we can incorporate prior knowledge into our models and gain insights into their decision-making processes. This has significant implications for fields such as autonomous driving and power grid inspection, where transparent machine learning is critical for a responsible deployment. We hope that our work inspires further research into the development of trustworthy machine learning methods.

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GENEOnet: A NEW MACHINE LEARNING PARADIGM FOR PROTEIN POCKET DETECTION BASED ON GROUP EQUIVARIANT NON EXPANSIVE OPERATORS

Giovanni Bocchi[a], **Alessandra Micheletti**[a], **Patrizio Frosini**[b], **Alessandro Pedretti**[c], **Carmen Gratteri**[d], **Filippo Lunghini**[e], **Andrea Rosario Beccari**[e], **Carmine Talarico**[e]

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Equivariant operators are proving to be increasingly important in deep learning, in order to make neural networks more transparent and interpretable. The use of such operators corresponds to the rising interest in the so called "explainable artificial intelligence", which looks for methods and techniques whose functioning can be understood by humans. In accordance with this line of research, Group Equivariant Non-Expansive Operators (GENEOs) have been recently proposed as elementary components for building new kinds of networks [2]. Their use is grounded in Topological Data Analysis (TDA) and guarantees good mathematical properties to the involved spaces, such as compactness, convexity, and finite approximability, under suitable assumptions on the space of data and by choosing appropriate topologies.

In this talk we will show promising results obtained by applying GENEOs to an industrial problem, namely protein pocket detection [3]. Protein pockets detection is a key problem in the context of drug development, since the ability to identify a small number of potential binding sites, allows to speed up drug discovery procedures. In this talk we will show how GENEOs can be used to build a geometrical machine learning method, able to detect protein pockets better than ML techniques already in use, but being based only on 17 unknown parameters.

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PHYSICALLY-INFORMED NEURAL NETWORKS FOR PROPAGATING ORBITS OF SPACECRAFT AND DEBRIS IN LOWER EARTH ORBIT

João Funenga[a,b] , **Marta Guimarães**[a,b] and **Claudia Soares**[a]

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Careful planning of the propellant used for satellites ensures they follow a set trajectory. Drag is a major force acting on a satellite; if not considered, it can cause position errors of up to hundreds of kilometers. Following orbital motion laws matching sparsely observed data is critical in improving predictions of a satellite' s position in the future. We use physically-informed neural networks [1] to bias the model toward predictions that follow the equations describing laws of physics in space. Orbit trajectories are not deterministic and can be influenced by multiple factors, such as drag or the reference area (related to the satellite' s attitude). Our results show constant error in propagation, in contrast to the full-dynamics state-of-the-art propagators, whose error increases exponentially with time. In this work, we proposed a physically-informed neural network approach to predicting the position of a satellite in space. Our results demonstrate that our approach is more accurate than state-of-the-art propagators, which suffer from exponential error growth over time. By biasing our model towards physical laws, we improved our predictions' accuracy, even when working with sparse data. This work has important implications for the design and operation of satellites, which rely on accurate position predictions to ensure their correct trajectory and function.

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MS 14

Organizers: Matthias Ehrhardt, Rafał Weron

Abstract This minisymposium is an activity of the ECMI Special Interest Group (SIG) on Computational Finance. The SIG was launched at ECMI-2014 in Taormina and (together with the ITN-STRIKE network (2013-2016)) organized several sessions of a minisymposium in Computational Finance.
The computational complexity of mathematical models employed in financial mathematics has witnessed a tremendous growth. Advanced numerical techniques are imperative for the most present-day applications in financial industry. The aim of this minisymposium is to present most recent developments of effective and robust numerical schemes for solving linear and nonlinear problems arising from the mathematical theory of pricing financial derivatives and related financial products.

	Wednesday
Room	CR 10 D
11:30-12:20	Chairperson: M. Ehrhardt
10:40-11:05	Daniel Sevcovic
11:05-11:30	Anna Clevenhaus
11:55-12:20	Matúš Padyšák
11:55-12:20	Martyna Zdeb
15:30-17:10	Chairperson: R. Weron
15:30-15:55	Felix Müller
15:55-16:20	Joanna Janczura
16:20-16:45	Jonathan Berrisch
16:45-17:10	Weronika Nitka

	Thursday
Room	CR 113
13:30-15:10	Chairperson: M. Wobben
13:30-13:55	Michael Trebing
13:55-14:20	Sarah Schleicher
14:20-14:45	Tomasz Weron
14:45-15:10	Simon Hirsch

	Friday
Room	CR 10 B
10:40-11:30	Chairperson: J. Janczura
10:40-11:05	Jarosław Gruszka
11:05-11:30	Cyril Izuchukwu Udeani

MULTIVARIATE PROBABILISTIC CRPS LEARNING WITH AN APPLICATION TO DAY-AHEAD POWER PRICES

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This paper presents a new method for combining multivariate probabilistic forecasts, taking into account dependencies between quantiles and covariates through a smoothing procedure that allows for online learning. Two smoothing methods are discussed: dimensionality reduction using Basis matrices and penalized smoothing. The new online learning algorithm generalizes the standard CRPS learning framework [1] into multivariate dimensions. It is based on exponential weighted averaging and yields optimal asymptotic learning properties. We provide an in-depth discussion on possible extensions of the algorithm and several nested cases related to the existing literature on online forecast combination. The methodology is applied to forecast day-ahead electricity prices, which are 24-dimensional distributional forecasts. For robustness, we report the results of two alternative weighting schemes, the uniform combination, and relevant special cases.

The proposed method yields significant improvements over the uniform combination in terms of continuous ranked probability score (CRPS). We discuss the temporal evolution of the weights and hyperparameters and present the results of reduced versions of the preferred model. A fast C++ implementation of the discussed methods is provided in the R-Package profoc.

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A STUDY OF THE EFFECTS OF DIFFERENT BOUNDARY CONDITIONS ON THE VARIANCE OF THE HESTON MODEL

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The novel space mapping approach for the well-known Heston model leads to a fast calibration of the parameters to real market data. In the space mapping framework, a coarse and inexpensive calibration is performed by a gradient descent algorithm. The gradient descent algorithm uses the Heston PDE and the corresponding formal adjoint PDE.

The well-posed solution of the parabolic PDE requires the proper definition of an initial condition and boundary conditions. The boundary conditions for the asset are directly derived from the market assumptions. There are different approaches for the variance boundary conditions, as there are some challenges, e.g., the singularity of the PDE when the variance approaches zero.

The challenge of finding the right boundary condition is often avoided by using large spatial domains, highly non-uniform grids, as well as windowing. These techniques are not practical for us because they increase computational complexity and the gradient is calculated from the entire domain. Therefore, the different boundary conditions have a large direct impact on the algorithm.

This work focuses on this sensitive part of the algorithm. We discuss various boundary conditions and present a strategy to reduce the impact of the boundary conditions for the gradient descent algorithm.

PORTFOLIO OPTIMISATION VIA THE HESTON MODEL CALIBRATED TO REAL ASSET DATA

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The debate between active and passive investment strategies has been ongoing for many years and is far from being over. During the talk we will show our latest results, which confirm that the choice of an optimal portfolio management strategy depends on an investment climate, which can measured via the parameters of the Heston model calibrated to the real stock market data. Depending on the values of those parameters, the passive strategy may outperform the active ones or vice versa. The method is tested on three stock market indices: S&P500, DAX and WIG20 [1].

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MULTIVARIATE SIMULATION-BASED FORECASTING FOR INTRADAY POWER MARKETS: MODELING TIME-VARYING DEPENDENCE AND CROSS-PRODUCT PRICE EFFECTS

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Intraday electricity markets play an increasingly important role in balancing the intermittent generation of renewable energy resources, which creates a need for accurate probabilistic price forecasts. However, research to date has focused on univariate approaches, while in many European intraday electricity markets all delivery periods are traded in parallel. Thus, the dependency structure between different traded products and the corresponding cross-product effects cannot be ignored. We aim to fill this gap in the literature by using copulas to model the high-dimensional intraday price return vector. We model the marginal distribution as a zero-inflated Johnson's S_U distribution with location, scale and shape parameters that depend on market and fundamental data. The dependence structure is modelled using latent beta regression to account for the particular market structure of the intraday electricity market, such as overlapping but independent trading sessions for different delivery days. We find that the correlation depends non-linearly on trading time and structural market elements such as the coupling of cross-border order books. We validate our modelling approach in a simulation study for the German intraday electricity market. However, the approach is directly applicable to other European electricity markets.

Acknowledgments Simon Hirsch gratefully acknowledges support from Statkraft.

EXPECTILE-BASED FORECASTING OF ELECTRICITY PRICES

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We propose new approach for deriving probabilistic forecasts of electricity prices. To this end, we utilize the notion of expectiles, originally introduced in [1]. Expectiles can be determined as the minimizer of an asymmetric least squares criterion:

$$\mu_\tau = \arg\min_{\mu\in\mathbb{R}} \tau\mathbb{E}[(X-\mu)_+^2] + (1-\tau)\mathbb{E}[(X-\mu)_-^2]$$

and can be viewed as an alternative specification of a distribution to quantiles. On the other hand, there is a functional relation between quantiles and expectiles [2]. Hence, expectiles of a predicted distribution can be used for least squares estimation of the corresponding quantiles, i.e. prediction intervals. We use three different approaches to derive probabilistic forecasts of electricity prices: i) direct calculation of quantiles; ii) calculation of quantiles from the expectiles; iii) calculating expectiles on a level corresponding to a given quantile. Prediction intervals are calculated for the day-ahead electricity prices for the EPEX market. Accuracy of the predictions is then compared in terms of the pinball score. The obtained results show that deriving prediction intervals from expectiles of the forecasted distribution of electricity prices outperforms the standard quantile-based approaches.

Acknowledgments The work was financed by the National Science Center (NCN, Poland) under Sonata grant nr. 2019/35/D/HS4/00369.

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UNLOCK POTENTIALS FOR THE ENERGY TRANSITION - OPTIMIZE GRID MAINTENANCE

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The energy transition requires a reliable and efficient electrical grid infrastructure to support the integration of renewable energy sources. However, aging equipment, increasing demand, and environmental challenges make it difficult for grid operators to maintain a high level of reliability. Traditional grid maintenance practices based on predetermined schedules or reactive responses to failures are no longer sufficient. In this talk, we present a mathematical and machine learning approach to identify risky assets and hence, optimize the grid maintenance strategy. We propose a data-driven approach that leverages historical failure data, monitoring and asset data to predict potential failure locations and time windows. We present the results based on our project work with a grid operator, demonstrating the effectiveness of our methodology in optimizing grid maintenance. Our work provides a practical approach for grid operators to unlock the full potential of their grid infrastructure for the energy transition.

MANAGING MARKET RISK FOR A SMALL RENEWABLE ENERGY GENERATOR USING BOOTSTRAP-BASED FORECASTS

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A small renewable energy utility, e.g. a wind farm, is susceptible to multiple sources of business risk. They operate in the electrical energy market, where prices tend to be highly volatile. Additionally, contrary to conventional power plants, the amount of energy they may produce is intermittent and subject to uncertainty. In this work we aim to support the decision-making process of such a utility by proposing a data-based approach for planning market bids. The goal of this algorithm is to mitigate these financial risks by optimizing the amount of energy offered in day-ahead market.

In this simulation study, we propose and apply a novel autoregressive bootstrap-type model to produce joint probabilistic forecasts of day-ahead and intraday market prices and wind energy generation. Basing on such forecasts, we establish a number of strategies which an utility may use to decide their market bids, depending on their risk tolerance. We evaluate financial impact in terms of value at risk and expected income of applying the proposed strategies for a model company operating in EPEX SPOT market. We show that the proposed methods can be successfully used to make data-driven business decisions.

BOND TRADING STRATEGIES USING MACHINE LEARNING TECHNIQUES

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Corporate bonds, on average, have a higher probability of default than government bonds, which are often regarded as risk-free investments. Consequently, investors require higher returns for holding riskier bonds compared to government bonds issued by countries like Germany or the US, which are commonly considered risk-free. In practice, the yields of riskier bonds consist of a risk-free component and an additional spread as compensation for the increased risk. However, market prices are constantly changing due to supply and demand dynamics and market participants' risk appetite or aversion. As a result, mark-to-market bond prices continuously fluctuate, which can lead to significant profits or losses when bonds are sold before maturity.

Increased risk appetite or demand for safe assets can cause daily returns for government and corporate bonds to differ significantly, especially during market stresses or recoveries. These differences raise the question of whether it is possible to time exposure to government and corporate bonds in order to achieve higher profits compared to, for example, investing solely in one type of bond. Such strategies for deciding between risk-free and risky asset allocations are commonly studied in the literature and used in practice, but mainly for stock markets.

We predict daily returns of the European corporate bond markets using a penalized Lasso regression or Random Forests. These predictions are further utilized in investment strategies that allocate into risky positions defined as either interest-rate hedged corporate bonds or unhedged corporate bonds and risk-free positions in safe government bonds proxied by the Euro-Bobl or Euro-Schatz futures which track the German government bonds. The strategy invests in corporate bonds if the predicted return is positive and in government bonds if the predicted return is negative. Our strategies obtain higher returns compared to passive investing in corporate bonds, but the daily rebalancing can be costly in practice.

We examine transaction costs ranging from 1 to 5 basis points and identify the breakeven costs that would erode profits. Secondly, we suggest two approaches to mitigate the costs investors incur during trading. The first approach involves rebalancing if the predicted return exceeds the expected transaction costs. The second approach involves less frequent rebalancing.

Acknowledgments The work has been supported by VEGA 1/0760/22 project.

UNLOCK POTENTIALS FOR THE ENERGY TRANSITION - ANALYSIS OF GRID EXPANSION, RENEWABLES AND HYDROGEN WITH MATHEMATICAL OPTIMIZATION

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One of the key challenges of this century is the reduction of greenhouse gas emissions in the energy sector. The required transition raises new questions concerning the entire energy system. These include, for example, the increasing role of sector coupling (the linking of the energy sector with the transport, residential heating/cooling and industry sector), the role of hydrogen in a climate-neutral energy system, the optimal expansion of renewable energies and the evaluation of grid expansion options. High-resolution energy system models and mathematical optimization provide tools to address these issues and can be used to study the potential impact of different recommendations for action. In this talk, we provide insights into possible use cases for energy system modeling and the mathematical problem. In addition, we address some mathematical challenges from our daily project work.

APPLICATION OF MAXIMAL MONOTONE OPERATOR METHOD FOR SOLVING HJB EQUATION ARISING IN OPTIMAL PORTFOLIO SELECTION

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The purpose of this talk is to investigate a fully nonlinear evolutionary Hamilton-Jacobi-Bellman (HJB) parabolic equation utilizing the monotone operator technique. We consider the HJB equation arising from portfolio optimization selection, where the goal is to maximize the conditional expected value of the terminal utility of the portfolio. The fully nonlinear HJB equation is transformed into a quasilinear parabolic equation using the so-called Riccati transformation method. The transformed parabolic equation can be viewed as the porous media type of equation with source term. Under some assumptions, we obtain that the diffusion function to the quasilinear parabolic equation is globally Lipschitz continuous, which is a crucial requirement for solving the Cauchy problem. We employ Banach's fixed point theorem to obtain the existence and uniqueness of a solution to the general form of the transformed parabolic equation in a suitable Sobolev space in an abstract setting. Some financial applications (see [1,2]) of the proposed result are presented in one-dimensional space.

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POWER PRODUCTION PLANNING WITH QUANTUM COMPUTERS

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Many variants of the Unit Commitment Problem (UCP) framework for cost-efficiently planning the production of electric energy given a predicted demand can be formulated as mixed-integer problems. These can be solved efficiently with contemporary solver software on classical computers in deterministic cases. With today's energy supplies evolving towards a more decentralized structure, however, planning can be expected to become a lot more demanding in the future. Moreover, as energy production from renewable sources, which can only be predicted with limited precision, gains in importance, an increasing need for rapid discovery of robust solutions that perform well under a variety of circumstances can be anticipated. With these developments in mind, it appears natural to try to exploit the assumed capabilities of quantum computers in finding optimal states in large unstructured solution spaces.

We present a model for the UCP on quantum computers that can treat any number of power facilities and time steps, using a cost function composed of commitment and discrete dispatch costs. Lower and upper limits are placed on the power output from each running facility and there are requirements to remain in the running or paused state for a certain amount of time once entered.

For practical purposes and in the context of uncertain residual demand, identifying the perfect solution for one particular scenario may be less important than deriving plans that have a high chance to perform well given a known distribution of demand values. Due to the noisy behaviour of quantum computers, algorithms are usually performed a large number of times, producing a variety of solution states. We explore ways to take the samples produced by D-Wave quantum computers as candidates which can be evaluated against a sample from the demand distribution. This appears to be a promising approach for finding robust solutions at little additional cost.

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BOOTSTRAP-BASED FORECASTS IN BATTERY CHARGING STRATEGIES

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Nowadays more and more renewable energy sources (RES) emerge across Europe. Their most important advantage over the conventional ones –little to no environmental pollution. What is healthy for our planet however, is not necessary beneficial for energy markets. With their volatility and uncertainty of generation, RES greatly destabilize power grids. To address this issue energy storage systems, such as batteries, are becoming more common. Such installations not only provide safety but offer new trading possibilities as well. Although they main role is to ensure stability, batteries can also be used to buy energy when the price is low, store it, and then sell it –when high.

In this study, we propose a new autoregressive bootstrap approach to provide probabilistic forecasts of day-ahead market prices. Utilizing them, we develop several trading strategies. Within them, we participate in the trade only if a specified relation (depending on the strategy we follow) between forecasted daily maximum and minimum is satisfied. We use German, Spanish and Danish market data to evaluate our methods. We show that our approach can outperform simple autoregressive models in terms of Value-at-Risk and average profit per trading day.

Acknowledgments T. W. and K. M. were supported by the National Science Center (NCN, Poland) through grant no. 2019/34/E/HS4/00060.

LEARNING THE SOLUTION OPERATOR OF HAMILTON JACOBI BELLMAN EQUATIONS USING PHYSICS-INFORMED DEEPONETS

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Several differential equations from many scientific and engineering fields for modeling physical phenomena are analytically intractable, especially in high-dimensional space. Traditional numerical methods, including neural network approaches, have been extensively used to approximate solutions of such differential equations. Although some machine learning approaches, such as physics-informed neural networks, are faster than the conventional numerical methods; however, a slight change in the underlying parameters governing the differential equation could result in the retraining of the model. Therefore, in this study, we employ the physics-informed DeepONet (PI-DeepONet) [1] to approximate the solution operator of a fully nonlinear partial differential equation arising from finance. PI-DeepONet incorporates known physics into the neural network, which consists of a deep neural network that learns the solution of the PDE and an operator network that enforces the PDE at each iteration. We consider a fully nonlinear Hamilton–Jacobi–Bellman (HJB) equation arising from the stochastic optimization problem [3], where the goal of an investor is to maximize the conditional expected value of the terminal utility of a portfolio. The fully nonlinear HJB equation is first transformed into a quasilinear parabolic equation using the Ricatti transform [2]. Then, the solution of the transformed quasilinear equation is approximated using PI-DeepONet.

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PRICING OF INSURANCE-LINKED SECURITIES: A MULTI-PERIL APPROACH

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Every year we observe an increasing number of natural catastrophes striking different regions of the world. They cause enormous losses in property and infrastructure and are a cause of death and health loss of many people. There is a need for new natural catastrophe risk management techniques and new financial instruments that could be used as protection from potential catastrophe risks.

At the moment, insurance-linked securities are widely used for that purpose. Most of the available literature deals with catastrophe instruments based on one kind of hazard affecting one region at a time. As regions might usually be affected by more than one type of natural catastrophe and catastrophes usually affect several nearby regions, there has been recent interest in creating and pricing of multi-region and multi-peril catastrophe securities.

One of the most often issued insurance-linked securities are catastrophe bonds and they will be our main interest during the talk. Issuance of a catastrophe bond allows the company to collect funds for possible losses connected with natural catastrophe. If the bond is triggered by the occurrence of specified event, the company can use collected funds to cover the losses and may be partially or entirely released from the obligation to pay the principal of the bond back to the investors.

During the presentation, we will first discuss modelling of the aggregate loss process for natural catastrophes. Next, we will focus on the construction and pricing of proposed multi-peril and multi-region catastrophe bonds.

MS 15

Organizers: Matti Heilio, John Mango, Bengt Ove Turesson, Verdiana Masanja, Poul Hjorth, Guttorm Alendal

Abstract Universities of Linköping and Uppsala have a long history of collaboration in the East African region. The PhD program touched areas running from agri-business, fish farms, traffic congestion, search engines to inverse problem in heat measurements and tumor localization plus many other topics in Mathematics.
Lappeenranta has coordinated projects focusing on academia-industry-society outreach. In 2022 a Mathematical Study Group and a Modelling Week were organized. ECMI contributed by a key resource person. The ongoing Norad supported project MATH4SDG by University of Bergen will be reported.

	Friday
Room	CR 10 D
10:40-11:05	John Mango
11:05-11:30	Matti Heilio
11:55-12:20	Poul Hjorth
11:55-12:20	Guttorm Alendal

FINNISH PROJECTS IN EASTERN AFRICA. OUTREACH TO STAKEHOLDERS

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[b]Nelson Mandela African Institute of Science and Technology, Tanzania

There has been steady collaboration Finland-Eastern Africa 2004-2015. The first projects were: East Africa Technomathematics I-IV and Mathematics Education and Working Life Relevance in East Africa. The content was student exchange, staff visits, intensive courses and thematic workshops. Also three Modelling Weeks were organized; hence introducing the ideas of modelling and real world related approach in MS curriculum. Recent and ongoing activities are Applied mathematics double PhD school, remote sensing and epidemiology (AMARE), LUT-AIMS-University of Rwanda 2021-2023, and Working life interaction in modelling and data skills (Wolimods), TFK-programme 2022-2024.

The ongoing project is a concerted capacity building program of awareness building, outreach to industry and stakeholder organizations, problem solving workshops and training of PhD students. African PhD students are recruited for a collaborative PhD training. The trainees will acquire skills of data-tools, software for simulation, data-analysis, advanced modelling tasks. This will encourage to seek employment in industrial R&D. First East –African Study Group was organized in October 2022 at Nelson Mandela African Institute of Science and Technology. The problems submitted to the Study Group were a result of outreach of professor Verdiana Masanja and her pioneering role in building contacts to stakeholders. We will hear her live report about the effort via Internet.

There will be a separate talk about the Study Group experience by Poul Hjorth. The next phase of the project was a Modelling Week for Masters students at University of Dar es Salaam, December 2022. About 35 students from three universities attended and tried their skills on 6 real life problems.

A STUDY GROUP IN EAST AFRICA

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In October 2022 a Study Group with Industry was conducted at the Nelson Mandela African Institute for Science and Technology (NM-AIST) in Arusha, Tanzania. The event was part of an ongoing effort to strengthen industrial mathematics in the East Africa region. Local academics, local Ph.D. students, and a few European researchers [1] took part on the academic side. Three industrial partners presented problems: TAFORI (on forestry modelling), TANESCO (on power line energy distribution), and NIMR (on public health policies). In this brief talk I will describe the settings for the workshop, the problems, and the preliminary analysis which the study group participants arrived at.

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THE HEAVY PHD TRAINING IN APPLIED MATHEMATICS AT MAKERERE UNIVERSITY UNDER SIDA SUPPORT 2015-2022

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It all significantly started in 2015 when Sida committed 39M SEK to a project 'Capacity Building in Mathematics and its Applications' under the Sida bilateral program with Makerere University 2015-2020, extended to 2022. Twenty one PhD students and 7 postdocs were trained. In the present symposium, we present the research topics of industrial applications taken by the PhD students and the postdocs. The results obtained and the iterations with industries in the course of training. Challenges faced with the interaction with local industries are further highlighted. Suggestions for further interaction of mathematicians and the local industries are further discussed. A hint on the origin of heavy support by Sida is given.

MS 16

Organizers: Tim Myers, Francesc Font

Abstract The European Green Deal involves a set of proposals designed to reduce climate change and environmental degradation. The proposals are also aligned to the UN Sustainable Goals and concern topics such as the reduction of greenhouse gases, removal of environmental toxins, biodiversity, energy efficient buildings, healthy food and renewable or recycled products. In this minisymposium we will address a number of these issues, with the ultimate aim of using mathematics to improve the environment. In the first session we focus on a standard method for environmental contaminant removal, namely adsorption, in the second we look into a broader range of environmental topics.

	Friday
Room	CR 10 AC
10:40-11:05	Tim Myers
11:05-11:30	Maria Aguareles
11:55-12:20	Francesc Font
11:55-12:20	Lucy Auton
15:30-15:55	Ellen Luckins
15:55-16:20	Marc Calvo-Schwarzwalder

DYNAMICS OF A SIPS-BASED MODEL FOR COLUMN ADSORPTION

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In this talk we investigate the dynamics of a contaminated fluid flowing through an adsorption column. We derive a one dimensional advection-diffusion equation coupled to a sink term that accounts for the contaminant adsorption. The adsorption rate is modeled by the Sips equation, where the order of the exponents is obtained from the chemical reaction. We apply different techniques to reduce the complexity of the governing equations which in some parameter limits allow to obtain explicit expressions for the concentration at the outlet of the reactor. These solutions are verified against the numerical resolution of the whole system of partial differential equations as well as with experimental data showing excellent agreement. The simplicity of these expressions is of great importance to adsorption column designers. The results to be presented can be found in [1] where, for the first time, analytical solutions for sink terms beyond the standard Langmuir and Linear Driving Force models are provided.

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DECONTAMINATING DRINKING WATER: MATHEMATICAL MODELLING OF FLUORIDE REMOVAL FILTERS

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Two key challenges that if tackled can drastically improve sustainability are removing pollutants from waste products of industrial processes to prevent them contaminating our air or water and decontaminating our existing resources, especially in regions of high demand but low availability. Despite the importance such filters, models which accurately account for the chemical mechanisms by which the contaminant is removed are often lacking. Commonly, Langmuir removal is assumed and this frequently has poor agreement with experiments because it is not describing the complex chemical reactions which occur within the filter. Here, we develop a model that captures the dominant chemical mechanisms involved in the removal of fluoride from water by a novel adsorbent designed by our experimental partners in IIT Kharagpur. These filters which comprise a mixture of mineral rich carbon (MRC) and chemically treated mineral rich carbon (TMRC), have been commercialised and are being purchased by the India government and deployed across rural India to aid in the decontamination of the scarce fresh water supplies. Working with experimental data from IIT Kharagpur, we develop and subsequently validate a mathematical model for both the MRC and the TMRC based on the underlying chemical reactions between the contaminant and the adsorbents. Even though the filters comprise a 1:40 ratio of TMRC to MRC, we find that the TMRC dominates the removal but that the MRC does play a role in early and late times. Development of a model which accounts for the complex chemistry occurring in such a filter will enable us to accurately predict the effect of geometrical changes of the filter and thus optimise the design of these fluoride removal filters to increase efficacy, increase longevity and decrease cost, which will subsequently enable more people to access safe drinking water.

MATHEMATICAL MODELLING OF HYDROGEN STORAGE IN METAL HYDRIDES

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A major concern to be addressed to make hydrogen technology viable is the safe storage of hydrogen in vessels with the desirable weight, volume and cost. Hydrogen stored as an adsorbed element inside metal hydride materials offers several advantages compared to high-pressure gaseous or cryogenic storage systems in terms of compactness, storage at conditions close to ambient, as well as being inherently safe because the hydrogen is stored at low pressure.

Previous research efforts towards the mathematical description of hydrogen storage in metal hydrides have focused on 2D/3D computational models and averaged 1D models are almost inexistent. In this talk, we will formulate a 1D averaged mathematical model for hydrogen storage in a metal hydride tank. The model consists of a set of governing equations describing gas flow and heat and mass transfer with appropriate source/sink terms characterising the sorption of hydrogen in the metal [1]. Solutions to the model will be presented and compared with experimental data. We will conclude by discussing possible routes to improve the model and its potential application as a tool to predict the state of charge of a metal hydride tank.

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MULTISCALE MODELLING OF DRYING SOIL AND ROCK

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There are many important environmental motivations to better understand the drying of soils and rock. For instance, we would like to be able to predict the effect of changing climates on agricultural soil moisture, understand the weathering of rock due to deposition of salts during drying, and learn how best to harness the heat losses to evaporation from soil as a cooling mechanism in green roofs. The drying of porous soils and rocks is generally difficult to model due to the multi-scale nature of the transport and phase change in the porous structure. In this talk we show how asymptotic methods may be used to derive effective drying models that accurately but efficiently capture the multi-scale evaporation processes [1]. In particular, we present a model for the coupled motion of an evaporation front through rock and the deposition of salts and impurities left behind during the drying. Using this model, we can compute deposition profiles of the salt and identify mechanisms by which the deposition can clog the rock, inhibiting further evaporation.

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USING MATHEMATICS TO IMPROVE THE DESIGN OF ADSORPTION COLUMNS

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Adsorption columns are employed in greenhouse gas capture, water treatment and groundwater remediation, biogas cleansing, chromatography and the purification of biopharmaceutical products. Industrial uses include: water providers (removing pollutants, odours, softening hard water and reducing evaporation); the cleansing of flue gases (for example from power stations, concrete and steel plants, pulp mills); biofuel purification; biotechnology companies; the paint/coating industry (to remove volatile fumes) and many more. Research in these fields is focussed on optimising the process, through the use of new adsorbents, configurations and operating parameters.

In this talk we describe the development and analysis of an array of mathematical models for column adsorption (setting up later talks in the minisymposium). The analysis involves coupling an advection-diffusion equation to a kinetic model describing mass loss. Approximate solutions are obtained through non-dimensionalisation, to identify negligible terms, and employing a travelling wave substitution. We also highlight errors in the current literature which invalidates many thousands of studies in the field and comparisons with data [1]. We demonstrate how these common errors have prevented the use of mathematical models to advance the understanding of adsorption and how the new, verifiable models can aid in the design of future adsorption equipment.

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THERMAL MANAGEMENT OF GREEN ROOFS

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Green roofs are a cost-effective, environmentally friendly solution to counteract the effect urban heat island effect, which is a great concern for residents and local authorities as they can have various public health implications, including mortality. Green roofs have been shown to reduce the heat island effect as they provide shade, remove heat from the air, and decrease temperatures of roofs and the surrounding air [1].

As discussed in [2], modelling heat transfer in green roofs is complicated due to the various layers involved and the movement of moisture. Here we develop a simple mathematical model to estimate the energy stored in a green roof and provide analytical solutions for extensive (shallow) and intensive (deep) substrates. Results are presented for the surface temperature and energy stored in both green roofs and concrete during a typical day. Within the restrictions of the model assumptions the analytical solution demonstrates that both energy and surface temperature vary linearly with fractional leaf coverage, albedo and irradiance, while the effect of evaporation rate and convective heat transfer is non-linear. We show that a typical green roof is significantly cooler and stores less energy than a concrete one even when the concrete has a high albedo coating. Evaporation of even a few millimetres per day from the soil layer can reduce the stored energy by a factor of more than three when compared to an equivalent thickness concrete roof [3].

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MS 17

Organizers: Joachim Linn, Dietmar Hömberg

Abstract The digital factory represents a network of digital models and methods for simulation and visualisation for the holistic planning, realisation, control and ongoing improvement of all factory processes related to a specific product. Within the last decade all industrialised countries have launched initiatives to realise this vision, sometimes also referred to as Industry 4.0 (in Europe) or Smart Manufacturing (in the United States). The goal of this minisymposium is to highlight recent developments in this area. The minisymposium is organized by the ECMI Special Interest Group MaDiFa (Math for the Digital Factory) bringing together university mathematicians working in modelling, simulation and optimization related to manufacturing and production with practitioners from industry in these areas. The general scientific goal is to develop a holistic mathematical view on virtual product development and MSO for manufacturing and production processes.

	Monday
Room	CR 10 D
15:30-15:55	Nina Kliche
15:55-16:20	Benjamin Bauer
16:20-16:45	Joachim Linn
16:45-17:10	Dietmar Hömberg

REAL-TIME APPROXIMATION OF NON-UNIFORM DISC PACKING PROBLEMS

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Packing problems have been widely studied in the optimization literature due to their various fields of application such as manufacturing, logistics, and transportation [1]. The vast majority of research papers focuses on creating optimal solutions to these NP-hard problems. Therefore, most literature methods are not suitable for human-interactive software, where efficiency and practicality are crucial factors. This contribution proposes an approximation method and a further heuristic for the problem of packing discs into a circular container of minimal radius.

The first approach is an incremental greedy-type algorithm that iteratively adds circles sorted by descending radii. Given a packing of at least two discs, each circle at the packing boundary may be viewed as vertex of a closed polygon. Then, every edge represents a pair of circles at which a third one may be packed deterministically. Choosing the optimal edge with respect to container size immediately yields a polynomial complexity of this fast procedure.

The second concept mainly picks up on the disc packing problem being a superposition of local continuous and global discrete optimization. In an offline phase we transform academic benchmarks [2] to their uniform version by shrinkage of radii and local optimization, but keep the circles digitally sorted by their former non-uniform radii. This creates a mapping of new non-uniform radii to the circles, which poses an effective heuristic for the global part of the problem. Thus, a single local optimization step in the online phase suffices to compute a decent approximate solution.

We evaluate the performance of the two algorithms on a set of academic benchmark instances and compare them with a state of the art method from literature [3]. Our experiments show that the greedy-type approach outperforms all other methods in terms of computational time by far. While it keeps up with the results of the compared method for most of the benchmarks, there are specific exception cases for which the container size is severely overestimated. We show how to detect and resolve these cases both meaningfully and efficiently. The lookup approach is much more robust due to the included optimization step, which vice versa leads to higher runtimes – particularly for large packings.

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TWO-SCALE TOPOLOGY OPTIMIZATION - A PHASE FIELD APPROACH

Dietmar Hömberg

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Subject of my presentation is a novel approach for optimizing both the macroscopic shape and the porous mesoscopic structure of components [1]. In the first part of my presentation I will introduce the concept of phasefield based topology optimization.

The second part of my presentation is devoted to two-scale topology optimization. The key feature here is the introduction of an additional local volume control (LVC), which allows to adjust the desired spatial scales.

The main novelty is that the radius of the LVC may depend both on space and a local stress measure. This allows for creating optimal topologies with heterogeneous mesostructures enforcing any desired spatial grading and accommodating stress concentrations by stress dependent pore size.

I will present some analytical results for the resulting optimal control problem and conclude with numerical results showing the versatility of our approach for creating optimal macroscopic designs with tailored mesostructures.

Joint work with Moritz Ebeling-Rump and Robert Lasarik, WIAS.

References

1. Moritz Ebeling-Rump, Dietmar Hömberg, Robert Lasarzik, *Two-scale topology optimization with heterogeneous mesostructures based on a local volume constraint.* Computers & Mathematics with Applications, **126** (2022), 100–114.

A NUMERICAL APPROACH FOR THE OPTIMAL OPERATION OF MINI-GRIDS UNDER UNCERTAINTY

René Henrion[a], **Dietmar Hömberg**[a] and **Nina Kliche**[a]

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Aiming at ensuring access to energy in countries where electrification is at low speed, mini-grids offer a reliable and affordable solution. Mini-grids are small scale power systems with decentralized energy generation sources that distribute energy through a local network. Renewable energy generation, demand and weather naturally introduce uncertainties whereas the installation of a battery energy storage system asks for consideration of battery degradation. As thermal issues can significantly affect battery lifetime, an optimal control problem for the daily operation including battery thermal management using a battery and temperature model [1] under uncertainties is set up and a numerical approach [2] is presented.

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MODELLING AND SIMULATION OF INELASTIC CONSTITUTIVE BEHAVIOUR: 2D COSSERAT RODS AND HYSTERESIS OPERATORS

Davide Manfredo[a,b] , **Vanessa Dörlich**[a] , **Joachim Linn**[a] and **Martin Arnold**[b]

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Due to their complex structure and different materials used, electric cables behave inelastically. In cyclic loading, open hysteresis loops can be observed, with noticeable difference between the first load cycle and the following ones. The mathematical theory of hysteresis represents a good choice to model and describe such complex behaviour. In this contribution, starting from a discrete two-dimensional Cosserat rod model [1], we present a procedure to include an inelastic constitutive law formulated in terms of a suitable hysteresis operator [2] in a 2D Cosserat rod model to perform quasi-static simulations.

On one hand, we consider a 2D Cosserat rod model, described by its centreline and rotation angle, for which the static equilibrium is found by minimising the elastic potential energy expressed as a function of shear-extensional strains and bending curvature, as well as specific effective stiffness parameters [3]. On the other hand, the Prandtl-Ishlinskii operator plays a relevant role in modelling the input-output relation in phenomena showing hysteretic behaviour and can be expressed as a superposition of elementary stop operators multiplied by a suitable weight function. By superimposing different elementary stop operators, one is able to model complex hysteresis effects taking into account the history of the process.

The approach foresees, firstly, to identify a suitable hysteresis operator able to capture the inelastic relation between bending moment and bending curvature. Secondly, we define a series of boundary conditions or constraints for each discrete time node, generally expressed in terms of positions and angles at both ends of the rod. Starting from an initial approximation of the bending stiffness, at each simulation step we change the bending stiffness value according to the hysteresis operator and the pre-curvature of the cable, hence we update the value of the simulated bending moment.

Acknowledgments This project has received funding from the European Union' s Horizon 2020 research and innovation programme under the Marie Sklodowska-Curie grant agreement No 860124.

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MS 18

Organizers: Anna Panorska, Agnieszka Wyłomańska

Abstract Stochastic models serve many science and engineering disciplines including hydrology, ecology, climate and environmental science, engineering, finance and actuarial science, and computer science. The models take into consideration the natural variability of the processes they describe and provide tools for description and prediction of the events of interest. The models we present have wide ranging applications which include processes with large variability and infinite variance. Such processes include precipitation, non-Gaussian signals observed in several engineering and science applications, currency exchange rates and insurance claims. The minisymposium aims to gather researchers interested in new mathematical ideas on analysis of such data.

	Wednesday
Room	CR 114
10:40-11:05	Anastassia Baxevani
11:05-11:30	Anna Panorska
11:30-11:55	Marek Arendarczyk
11:55-12:20	Tomasz Kozubowski
15:30-15:55	Aleksandra Grzesiek
15:55-16:20	Agnieszka Wyłomańska
16:20-16:45	Krzysztof Podgórski

THE GREENWOOD STATISTIC, STOCHASTIC DOMINANCE, CLUSTERING AND HEAVY TAILS

Marek Arendarczyk[a], **Tomasz J. Kozubowski**[b] and **Anna K. Panorska**[b]

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The Greenwood statistic T_n and its functions, including sample coefficient of variation, often arise in testing exponentiality or detecting clustering or heterogeneity. We provide a general result describing stochastic behavior of T_n in response to stochastic behavior of the sample data. The motivation for this work is the practical need to understand the behavior of the Greenwood statistic for samples from heavy-tailed distributions. Such distributions are often used as models for data with very large outliers originating in the environment, weather, climate or finance (e.g. flood, deluge, heat waves, extreme precipitation, draught, or large changes in the financial assets' prices), and other areas of interest. From practical perspective, extreme events are of primary importance for governments, safety and disaster response organizations, human health, and the economy. Mathematically, these events are studied in the Extreme Value Theory and Peak-Over-Threshold (POT) theory. Two of the main properties of interest in the study of extremes are clustering and heavy-tailed distributions, and we present mathematical and intuitive explanation of the connection between them for several classes of distributions. Our results provide theoretical justification for T_n being an effective and commonly used statistic discriminating between regularity/uniformity and clustering in presence of heavy tails in applied sciences.

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EFFECTIVE PROBABILITY DISTRIBUTION APPROXIMATION FOR THE RECONSTRUCTION OF PRECIPITATION DATA

Anastassia Baxevani[a], **Christos Andreou**[a] and **Dionissios T. Hristopulos**[b]

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Spatially distributed processes can be modeled as random fields. The complex spatial dependence is then incorporated in the joint probability density function. Knowledge of the joint probability density allows predicting missing data. While environmental data often exhibit significant deviations from Gaussian behavior (rainfall, wind speed, and earthquakes being characteristic examples), only a few non-Gaussian joint probability density functions admit explicit expressions. In addition, random field models are computationally costly for big datasets. We propose an *effective distribution* approach, [1] which is based on the product of univariate conditional probability density functions modified by local interactions. The effective densities involve local parameters that are estimated either by means of kernel regression or using origins equations. The prediction of missing data is based on the median value from an ensemble of simulated states generated from the effective distribution model. The latter can capture non-Gaussian dependence and is applicable to large spatial datasets, since it does not require the storage and inversion of large covariance matrices. We apply the effective distribution approach to the reconstruction of gaps in precipitation data. Precipitation modeling is particularly challenging due to intermittence, areas of high precipitation may be followed by areas of no precipitation. Compound Poisson gamma distribution, [2], is a model with an atom at zero, making it ideal for precipitation data. The compound Poisson gamma model, which arises as a Poisson sum of gamma independent and identically distributed random variables, has a very nice natural interpretation modelling the total precipitation as a sum of smaller events each one of them having the gamma distribution.

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TESTING OF TWO-DIMENSIONAL GAUSSIAN PROCESSES BY SAMPLE CROSS-COVARIANCE FUNCTION

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We address the issue of testing two-dimensional Gaussian processes with a defined cross-dependency structure. Multivariate Gaussian processes are widely used in various applications; therefore, it is essential to identify the theoretical model that accurately describes the data. While it is relatively straightforward to do so in a one-dimensional case, analyzing multi-dimensional vectors requires considering the dependency between the components, which can significantly affect the efficiency of statistical methods. The presented testing methodology is based on the sample cross-covariance function and can be considered a natural generalization of the approach recently proposed for testing one-dimensional Gaussian processes based on the sample autocovariance function. The efficiency of this procedure is verified on three classes of two-dimensional Gaussian processes: Brownian motion, fractional Brownian motion, and two-dimensional autoregressive discrete-time process. The theoretical and simulation results are supported by analyzing two-dimensional real-time series that describe the main risk factors of a mining company, namely copper price and exchange rates (USDPLN).

A UNIFORM LAPLACE MIXTURE DISTRIBUTION

Tomasz J. Kozubowski and **Amos Natido**

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We introduce a new stochastic model incorporating a mixture of uniform and Laplace distributions. We present basic theoretical properties of this model and discuss related computational issues of parameter estimation via expectation-maximization (EM) and moment-based computational schemes. We check the performance of the estimation algorithms on synthetic data and provide a data example related to renewable energy, illustrating modeling potential of this novel methodology.

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PRECIPITATION EXTREMES - ATMOSPHERIC RIVERS: PRESENT AND FUTURE

Anna Panorska[a] , **Marek Arendarczyk**[b] and **Tomasz Kozubowski**[a]

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We present results of current research on extreme precipitation. The model we describe is (X, Y, N), where X describes the magnitude, Y the maximum, and N the duration of events such as drought, heat wave, cold spell, extreme wind, or deluge. The distribution of the vector (X, Y, N) is of direct interest to water management, energy management companies, disaster management, health departments, environmental protection, as well as state and federal regulatory agencies. We present some very fresh results on the storms hitting the western US, with focus on the Atmospheric Rivers in California.

EMPIRICALLY DRIVEN SPLINE BASES FOR FUNCTIONAL PRINCIPAL COMPONENT ANALYSIS IN 2D

Rani Basna[a], **Hiba Nassar**[b] and **Krzysztof Podgórski**[a]

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Functional data analysis is typically performed in two steps: first, functionally representing discrete observations, and then applying functional methods, such as the functional principal component analysis, to the so-represented data. While the initial choice of a functional representation may have a significant impact on the second phase of the analysis, this issue has not gained much attention in the past. Typically, a rather ad hoc choice of some standard basis such as Fourier, wavelets, splines, etc. is used for the data transforming purpose. To address this important problem, we present its mathematical formulation, demonstrate its importance, and propose a data-driven method of functionally representing observations.The method chooses an initial functional basis by an efficient placement of the knots.

A simple machine learning style algorithm is utilized for the knot selection and recently introduced orthogonal spline bases – splinets – are eventually taken to represent the data. The benefits are illustrated by examples of analyses of sparse functional data. A new extension of the data driven bases to the 2D functional data will be presented and illustrated by examples.

In the functional data analysis aimed at dimension reduction for sparse data, the locality of the selected basis for data representation plays a fundamental role. This feature is represented by the wavelet and B-spline bases. Of the two, only the B-spline bases are flexible in representing different patterns of the locality at different locations if we allow a data-driven knot selection, see [1]. The B-spline basis is not orthogonal, which may lead to computational inefficiencies in representing data. In our recent work, we propose an efficient dyadic orthogonalization algorithm that leads to an orthogonal spline basis that preserves the locality of the B-splines. These bases are called splinets and implemented in an R-package for splines residing on either an interval or on a circle (the periodic case), see [2].

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FRACTIONAL BROWNIAN MOTION WITH CONSTANT AND RANDOM HURST EXPONENT - MATHEMATICAL FRAMEWORK AND STATISTICAL TESTING

Agnieszka Wyłomańska, **Aleksandra Grzesiek**

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It has been determined that anomalous diffusion behavior arises from fractional Brownian motion, the Gaussian process with self-similar property, in a wide range of physical systems. The Hurst exponent fully describes the correlation and diffusion aspects of this random motion. However, the class of self-similar random processes seems to be insufficient for complex anomalous diffusion phenomena that were discovered e.g. in recent single particle tracking investigations in biological cells. These discoveries led us to investigate the mechanism that, while maintaining the characteristics of fractional Brownian motion at a single trajectory level, causes the Hurst index to fluctuate erratically from trajectory to trajectory. For analytical, numerical, and statistical analysis of fractional Brownian motion with stochastic Hurst exponent, we present a general mathematical framework. In the simulation study we consider the example distributions of the Hurst exponent and demonstrate the specific behavior of the analyzed process. Finally, we propose a statistical methodology for discriminating the fractional Brownian motion with constant and random Hurst exponent by application the statistics of time-averages.

Acknowledgments The work is supported by the National Center of Science under Opus Grant 2020/37/B/HS4/00120 "Market risk model identification and validation using novel statistical, probabilistic, and machine learning tools".

MS 19

Organizers: Neil Budko, Wil Schilders

Abstract Industrial mathematics changes its focus in accordance with the current needs of the industry. This minisymposium gives a snapshot of topics that are trending in the Netherlands and elsewhere. We discuss the application of the digital twins technology in the electronics industry, numerical simulation of jets in co-flow, inverse methods for freeform optical design, and robust methods for ill-posed problems in agriculture.

	Wednesday
Room	CR 115
10:40-11:05	Jan ten Thije Boonkkamp
11:05-11:30	Domenico Lahaye
11:30-11:55	Wil Schilders
11:55-12:20	Neil Budko

INVERSE METHODS FOR FREEFORM OPTICAL DESIGN

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Inverse methods for freeform optical design compute the shape of an optical surface (reflector/lens) that converts a given source light distribution, typically LED, in a desired target distribution. The surface is referred to as freeform, as is has no symmetry. Applying the principles of geometrical optics, we can derive a geometrical description of an optical system, which for many systems can be formulated in terms of a so-called cost function as known from optimal transport theory. From this description we can subsequently derive a PDE for the optical map, connecting a point in the source domain with a point in the target domain. Combining this equation with energy conservation, we can derive a fully nonlinear PDE for the shape of the optical surface.
We have developed the following classification for optical systems [1,2]. First, the simplest optical systems, typically a reflector transferring a parallel source distribution in a far-field target distribution, can be described by a quadratic cost function, and the corresponding PDE for the optical surface is the standard Monge-Ampère equation. Second, for more complicated systems, such as a lens converting a point-source distribution in a far-field target distribution, the cost function is non-quadratic and the governing equation for the optical surface is a generalized Monge-Ampère equation. Finally, there are optical systems, typically for near-field target distributions, that no longer allow a description in terms of a cost function. Instead, a generalization in terms of a generating function is possible, and the corresponding PDE for the optical surface is a generated Jacobian equation.
We have developed least-squares solvers for all three classes of optical systems [2]. Our least-squares solvers for the Monge-Ampère equations are two-stage algorithms, i.e., in the first stage the optical map is computed, and in the second stage, the shape of the optical surface is reconstructed from the optical map. Both stages are least-squares solvers. The least-squares solvers for the generated Jacobian equation is a slight modification of these methods. Our algorithms can handle quite complicated source and target distributions, and are currently transferred to industrial production code. We will demonstrate the performance of our solvers for several examples.

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ROBUST METHODS FOR ILL-POSED PROBLEMS IN AGRICULTURE

Neil Budko

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Modern precision agriculture is mostly concerned with predicting the performance of crops in various environments and conditions. Construction of a predictive model usually involves large-scale experiments performed with selected genotypes in test fields where some important characteristics of the crop (phenotype) are measured, possibly, as functions of time. Then, the crop model is constructed, applying a range of machine-learning (ML) techniques. The cost and duration of field experiments in agriculture are high to an extent that the typical ML problem is often underdetermined, i.e., the number n of measurements of the phenotype variable that one wishes to predict is much smaller than the number p of potential explanatory variables (features), i.e., $n \ll p$. In addition, the measured data contain systematic and random noise, which makes the corresponding ML problem severely ill-posed.

In this talk we shall describe a project where the size of the canopy of a potato plant is predicted from the bio-chemical properties of the seed tuber. We demonstrate the difficulties one faces while constructing even the most simple iteratively-regularized linear model $y = X\beta + \epsilon$. In this iterative regularization method, the dimension of the Krylov subspace, reflected by the iteration count, plays the role of the regularizing factor. Validation cycle carried out with the data from the project systematically indicated that the optimal value of the iteration count is one, i.e., the regularized solution lives in a one-dimensional Krylov subspace.

Guided by these observations we propose an alternative ML approach by posing an *Inverse Regression* (IR) problem, where instead of recovering the scalar function of multiple variables $f : \mathbb{R}^p \to \mathbb{R}$ in the assumed model $y = f(x_1, \ldots, x_p) + \epsilon$, we recover the vector function of a single variable $\vec{f} : \mathbb{R} \to \mathbb{R}^p$ in the assumed "inverse" model $x_i = f_i(y) + \epsilon_i$, $i = 1, \ldots, p$. We show, in particular, that the linear version of this IR model has an explicit solution and is very similar to the one-dimensional Krylov subspace model described above, i.e., it is over-regularized and does not lead to overfitting. We shall also present a non-linear extension of the IR model.

Acknowledgments The work described here has been made possible through the financial support of the HZPC and Averis Seeds companies as well as the Rural Development Programme of the European Union.

NUMERICAL SIMULATION OF JETS IN CO-FLOW

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We wish to reveal how transient flow phenomena affect the performance industrial furnaces. Aspects such as turbulent mixing of gaseous fuel and oxidiser, radiative heat transfer and pollutant formation need to be taken into account. We therefore study the numerical simulation of a bluff-body stabilised jet flame in idealised settings. The extensively documented HM-1 test case is chosen as a test case. In this test case, the flow of fuel and oxidiser mixture fails to reach a steady-state. Unsteady phenomena in swirl combustion systems have been reviewed in the literature. Our goal here is to quantity using numerical simulation how the the unsteadiness affects the computed axial velocity, the radial velocity and the temperature in the HM-1 test case. The study of the impact on chemical species and radiative heat intensity is left to future studies.

In the HM1 test case, a gaseous fuel jet is injected through a centrally mounted pipe. The fuel is a mixture of 50 percent methane and 50 percent hydrogen. Ambient air as oxidiser is injected at room co-axially surrounding the fuel jet. The numerical simulation of the HM-1 has been pursued by various authors using both RANS and LES approaches for the flow and both eddy-dissipation and flamelet approaches for the combustion.

We perform simulations using an unsteady Reynolds-averaged Navier-Stokes (URANS) model closed by a k-ϵ turbulence model and standard wall functions. The combustion chemistry is model by an eddy-dissipation combustion with a one-step reaction model for both the methane and hydrogen fuel with known limitations. The radiative heat transfer is modelled by an P1 radiation model with mean-Planck coefficients. To avoid that an axi-symmetrical configuration constraints the nature of the flow, we perform simulations on a full three dimensional geometry.

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DIGITAL TWINS IN THE ELECTRONICS INDUSTRY

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Digital twins are a major subject of research and development in industry, and place a high demand on the mathematical methods needed for accurate and very efficient simulations. Digital twins are not "new" . In fact, it is a natural development: simulation evolved from a troubleshooting tool to key business driver in the form of digital twins. Up to a few years ago, simulation software was used to design and optimize products, but now we are going a step further by using the software also in operating environments. Thus, the designed product is monitored during its operation. But whereas in the design phase compute times are less important, the timing is extremely important in the operating phase. Indeed, having a true digital twin means that we need to be able to simulate the product or process in real time, or preferably even beyond real time. This requires extremely fast methods that can predict the behaviour, and use sensor data from the real product/process to obtain extremely accurate simulations that truly mimic the real device. Clearly, digital twins are also extremely important

in the electronics industry, and in this talk we will discuss various aspects of product development and operation in view of the digital twinning. Model order reduction is of the utmost importance, whereas accurate models of parameters can be provided by scientific machine learning.

MS 20

Organizers: Will Schilders, Toby van Gastelen, Lu Xia, Phillip Horn

Abstract Recently, the following two concepts have gained importance in computational science: (i) machine learning (in particular neural networks) and (ii) structure-preserving (mimetic or invariant-conserving) computing for mathematical models in physics, chemistry, astronomy, biology and more. While neural networks are very strong as high-dimensional universal function approximators, they require enormous datasets for training and tend to perform poorly outside the range of training data. On the other hand, structure-preserving methods are strong in providing accurate solutions to complex mathematical models from science. The goal of our research is to better understand neural networks to enable the design of highly efficient, tailormade neural networks built on top of and interwoven with structure-preserving properties of the underlying science problems that can serve as the simplified models mentioned above. This is unexplored terrain, and lead to novel types of machine learning that are much more effective and have a much lower need for abundant sets of data. In this minisymposium, we will present the project UNRAVEL and some recent results.

	Wednesday
Room	CR 115
15:30-15:55	Wil Schilders
15:55-16:20	Toby van Gastelen
16:20-16:45	Lu Xia
16:45-17:10	Philipp Horn

ENERGY-CONSERVING NEURAL NETWORK FOR TURBULENCE CLOSURE MODELING

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In turbulence modelling, and more particularly in the LES framework, we are concerned with finding a suitable closure model to represent the effect of the unresolved subgrid-scales on the larger/resolved scales. In recent years, the scientific computing community has started to gravitate towards machine learning techniques to attempt to solve this issue. However, stability and abidance by physical structure of the resulting closure models is still an open problem [1,2].

To resolve this, we take the discretize first and filter next approach starting out from a high-resolution reference simulation [3,4]. We apply a spatial averaging filter to reduce the degrees of freedom and derive a new kinetic energy conservation condition that takes into account both the resolved and unresolved scales. We then suggest a data-driven compression to represent the subgrid-scale content on the coarse grid in order to comply with our new conservation condition. Finally, a skew-symmetric convolutional neural network architecture is introduced that can be enhanced with dissipative terms to account for viscous flows. Combined with a structure-preserving discretization this framework is used to evolve both the filtered solution and the compressed subgrid-scale representation in time in a structure-preserving fashion, yielding non-linear stability, while still allowing for backscatter.

We apply the methodology to both the viscous Burgers' equation and Korteweg-De Vries equation in 1-D and show increased accuracy and stability as compared to a standard convolutional neural network. Furthermore, we consider the advection equation in 2-D where some quantity, e.g. a temperature distribution, is advected by atmospheric flows.

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A GENERALIZED FRAMEWORK OF NEURAL NETWORKS FOR HAMILTONIAN SYSTEMS

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When solving Hamiltonian systems using numerical integrators, preserving the symplectic structure is crucial [1]. At the same time, solving chaotic problems requires integrators to approximate the trajectories with extreme precision. This can be very computationally expensive. However, for example in [2] it was shown that a neural network can be a viable alternative to numerical integrators. Offering high accuracy solutions for the chaotic N-body problem many orders of magnitudes faster.

To understand when it is useful to add physics constraints into neural networks, we analyze three well-known neural network topologies that include a symplectic structure inside the NN architecture [3], [4]. Between these neural network topologies many similarities can be found [5]. This allows us to formulate a generalized framework for these topologies. With the new framework, we can find novel topologies by transitioning between the established ones.

We compare these new Generalized Hamiltonian Neural Networks (GHNN) against the already established SympNets and HénonNets and physics-unaware multilayer perceptrons. This comparison is performed with data from a pendulum, a double pendulum and a gravitational three-body problem. A special focus lies on the capability of the neural networks to generalize outside the training data. We found that the GHNN outperforms all other neural network architectures.

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THE UNRAVEL PROJECT: UNRAVELING NEURAL NETWORKS WITH STRUCTURE-PRESERVING COMPUTING

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The development of simplified computational models of complex fundamental phenomena in physics, chemistry, astronomy and biology is an ongoing challenge. The purpose of such simplified models is typically to reduce computational cost at a minimal loss of accuracy. At the same time, more importantly, these models can provide fundamental understanding of underlying phenomena.

Recently, the following two concepts have gained importance in computational science: (i) machine learning (in particular neural networks) [1,2,3] and (ii) structure-preserving (mimetic or invariant-conserving) computing for mathematical models in physics, chemistry, astronomy, biology and more [4,5,6]. While neural networks are very strong as high-dimensional universal function approximators, they require enormous datasets for training and tend to perform poorly outside the range of training data. On the other hand, structure-preserving methods are strong in providing accurate solutions to complex mathematical models from science.

The goal of the UNRAVEL project is to better understand neural networks to enable the design of highly efficient, tailor-made neural networks built on top of and interwoven with structure-preserving properties of the underlying science problems that can serve as the simplified models mentioned above. This is largely unexplored terrain, and will lead to novel types of machine learning that are much more effective and have a much lower need for abundant sets of data.

The resulting deeper understanding of neural networks from mathematical, physical and astronomical point of view is vital for future developments in this rapidly developing area.

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ON THE INFLUENCE OF STOCHASTIC ROUNDING BIAS IN IMPLEMENTING GRADIENT DESCENT WITH APPLICATION IN LOW-PRECISION TRAINING

Lu Xia[a], **Stefano Massei**[b], **Michiel E. Hochstenbach**[a], and **Barry Koren**[a]

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In the context of low-precision computation for the training of neural networks with the gradient descent method (GD), the occurrence of deterministic rounding errors often leads to stagnation or adversely affects the convergence of the optimizers [1,2]. The employment of unbiased stochastic rounding (SR) may partially capture gradient updates that are lower than the minimum rounding precision, with a certain probability [2,4]. We provide a theoretical elucidation for the stagnation observed in GD when training neural networks with low-precision computation. We analyze the impact of floating-point roundoff errors on the convergence behavior of GD with a particular focus on convex problems. Two biased stochastic rounding methods, signed-SR_ε and SR_ε, are proposed, which have been demonstrated to eliminate the stagnation of GD and to result in significantly faster convergence than SR in low-precision floating-point computation.

We validate our theoretical analysis by training a binary logistic regression model on the Cifar10 database and a 4-layer fully-connected neural network model on the MNIST database, utilizing a 16-bit floating-point representation and various rounding techniques. The experiments demonstrate that signed-SR_ε and SR_ε may achieve higher classification accuracy than rounding to the nearest (RN) and SR, with the same number of training epochs. It is shown that a faster convergence may be obtained by the new rounding methods with 16-bit floating-point representation than by RN with 32-bit floating-point representation.

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MS 21

Organizers: Idoia Cortes Garcia, Sebastian Schöps, Giovanni Mascali, Vittorio Romano, Iryna Kulchytska-Ruchka, Maria del Pilar Salgado Rodríguez, Maria Dolores Gomez Pedreira

Abstract Electrical engineering is an important technology for many recent societal and industrial developments. It includes the investigation and application of electrical engineering, electronics and semiconductors. Therein, scientific challenges are often driven by industrial needs and are related to classical and new emerging topics of applied mathematics and scientific computing, i.e., modeling, simulation, optimization, uncertainty quantification, stochastics and data analysis. This minisymposium is organized from within the ECMI SIG "Modeling Simulation and optimization in Electrical Engineering" . It contains two themes ("Low Frequency Electromagnetics" and "Mathematical Problems from Semiconductor Industry") that consist of three session each.

	Monday
Room	CR 10 AC
10:40-11:05	Maximilian Schade
11:05-11:30	Elias Paakkunainen
11:55-12:20	Idoia Cortes Garcia
11:55-12:20	Iván Martínez
15:30-15:55	Bernard Kapidani
15:55-16:20	Theodor Komann
16:20-16:45	Oscar Crego
16:45-17:10	Michael Mandlmayr
17:20-17:45	Bogdan Radu
17:45-18:10	Mario Mally
18:10-18:35	Nepomuk Krenn

	Tuesday
Room	CR 10 B
10:40-11:05	Vittorio Romano
11:05-11:30	Orazio Muscato
11:55-12:20	Giovanni Nastasi
11:55-12:20	Giorgia Vitanza
15:30-15:55	Giuseppe Alì
15:55-16:20	Patricio Farrell
16:20-16:45	Nella Rotundo
17:20-17:45	Francesco Vecil
17:45-18:10	Antonio Sellitto

CHARGE TRANSPORT IN 2D TRANSITION METAL DICHALGENIDES

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We derive a hydrodynamic model for charge transport in a 2D layer of MoS_2, based on the 6-moment equations of the electron distribution function in conduction band, using the parabolic band approximation, with the maximum entropy principle closure. We take into account the scattering of electrons with intravalley transverse and longitudinal acoustic phonons, with intervalley transverse and longitudinal acoustic phonons, with intravalley transverse optical phonons, with intervalley transverse optical phonons, with intervalley longitudinal optical phonons, with intervalley homopolar optical phonons, and the Fröhlich interaction with longitudinal optical phonons. All the closure relations for the spurious moments and the collision terms are explicitly evaluated. The proposed model is integrated numerically in the space-homogeneous case, with application to the computation of mobility.

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NUMERICAL SIMULATION OF INDUCTION FURNACES IN SISAL PILOT, AN INNOVATIVE PROJECT FOR SILICON PRODUCTION

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SisAl Pilot is a Horizon 2020 funded project aimed at demonstrating a patented, novel industrial process for silicon production. This more environmentally and economically sustainable alternative to the current carbothermic Submerged Arc Furnace (SAF) process involves aluminothermic reduction of quartz, which allows for the use of secondary raw materials instead of carbon reductants. During the project, different types of furnaces have been analysed. This talk will focus on the mathematical modelling and numerical simulation of induction heating furnaces. These models require the study of multiple physical processes, including heat transfer, multiphase fluid dynamics, electromagnetism, melting processes, and chemical reactions. The challenge is to develop simplified mathematical models capable of simulating the experimental trials and operational procedures performed in a plant by the industrial partners.

More precisely, the talk will focus on a thermoelectrical model that couples an eddy current problem with a transient heat transfer equation with phase change in axisymmetric domains. Among the challenges addressed, numerical tools to impose the source from the data known in a plant as the total power, modelling strategies for load changes throughout the simulation, or the treatment used for the phase change will be discussed.

Acknowledgments This project has received funding from the European Union' s Horizon 2020 research and innovation programme under grant agreement No 869268. This work has also received financial support from the Xunta de Galicia (2021 GRC GI-1563 - ED431C 2021/15).

MODELING AND NUMERICAL SIMULATION OF 2D MEMRISTIVE DEVICES

Patricio Farrell[a], **Benjamin Spetzler**[b], **Dilara Abdel**[a], **Frank Schwierz**[b] and **Martin Ziegler**[b]

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The von Neumann architecture is far from ideal for AI applications due to its unacceptably high energy consumption. Memristors help to emulate the energy efficiency of the human brain. We present complex charge transport models which incorporate sulphur vacancies and Schottky barrier lowering to theoretically understand the shape and asymmetries of the hysteresis curves observed in experiments. In particular, we can show the dominant role of the vacancies. The switching process is governed by the formation and annihilation dynamics of a local vacancy depletion zone. Moreover, minor changes in the interface potential barriers cause fundamentally different device behavior previously thought to originate from multiple mechanisms [2].

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INDEX AWARE LEARNING OF ELECTRIC NETWORKS

Peter Förster[a] , **Idoia Cortes Garcia**[a] , **Sebastian Schöpsb**[b] and **Wil Schilders**[a]

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Learning techniques such as Gaussian processes or neural networks can be employed to learn the (parameter dependent) solution of ordinary differential equations. However, electric circuits are typically described with the modified nodal analysis [1], which leads to a system of differential algebraic equations (DAEs). These systems often pose numerical difficulties that do not arise within ODEs. Therefore, not all methods designed for ODEs are immediately applicable to DAEs.

In this contribution, machine learning techniques that are usually employed to learn solutions of ODEs are adapted for their application to DAEs. In particular, it focuses on the appropriate treatment and decomposition of the different types of degrees of freedom arising within DAEs. This is done by means of the dissection index [2], a concept that allows for quantifiying the difficulty a given DAE conveys as well as its decoupling.

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ARBITRARY ORDER SPLINE APPROXIMATION OF TIME-HARMONIC EDDY CURRENT PROBLEMS AND COHOMOLOGY COMPUTATION IN THE CASE OF NON SIMPLY CONNECTED CONDUCTORS

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The eddy current problem has many relevant practical applications in science, ranging from non-destructive testing to magnetic confinement of plasma in fusion reactors. It arises when electrical conductors are immersed in an external time-varying magnetic field operating at frequencies for which electromagnetic wave propagation effects can be neglected: by virtue of Faraday' s magnetic induction law, electric current will develop in the conductor and induce an opposing magnetic field.

When numerical solutions are sought for the resulting total magnetic field through variational formulations, e.g. in the Finite Element Method (FEM), the most efficient strategy is through magnetic scalar potential based formulations in the non conducting parts of the spatial domain. These run into trouble when conductors present non-trivial topology, as the discrete approximation spaces must be then augmented with generators of the first cohomology group of the non-conducting domain. An automated solution for lowest order FEM has been provided in [1], where it was assumed that the extension of the graph-based algorithms to high-order approximations required hierarchical bases for the curl-conforming discrete spaces.

Building on seminal work on de Rham complexes approximation with splines [2], we will show in the present submission that the hierarchical basis condition is not necessary. The algorithms of [1] can instead be adapted to work on an underlying hexahedral mesh arising from isomorphisms between spline spaces of differential forms and co-chain complexes on an auxiliary control mesh, which was already exploited to gauge vector potential formulations in magnetostatics in [3].

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SHAPE AND PARAMETER OPTIMIZATION OF AN ELECTRICAL MACHINE WITH IGA

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Over the past decade, many prototypes were created, tested, and evaluated in the development of new electrical machines. Nowadays, virtual prototypes in the form of numerical models have largely replaced physical prototypes. It is therefore crucial to solve optimization problems based on such models efficiently. In this talk an efficient method for combining parameter and shape optimization within an Isogeometric Analysis (IGA) framework using the open-source software GeoPDEs is presented [1]. IGA employs Non-Uniform Rational B-Splines (NURBS) for exact geometry representation and eliminates the need for remeshing. This makes IGA suitable for shape optimization and compatible with CAD software, facilitating direct use of optimization results in design. Permanent Magnet Synchronous Motors (PMSMs) are described with sufficient accuracy by the magnetostatic approximation of Maxwell' s equations leading to a PDE constrained optimization problem. In this talk we will present a gradient based discretize then optimize approach for the design optimization of a 2D PMSM. The optimization variables consist of geometry parameters, e.g. length, width and position of the magnet as well as certain control points to vary other parts of the shape. The dependence of optimization parameters and control points is given by a black-box function. We compute the derivative of the objective function with respect to control points by using the adjoint method [2].The derivative of the control points with respect to the optimization variables is computed by finite differences, however, the derivative of the solution with respect to the control points is determined in closed form resulting in a significantly reduced computational cost. Since remeshing is not necessary, this procedure takes only a few milliseconds per geometric parameter, ensuring an efficient calculation. In the end we will present numerical results for the proposed approach.

Acknowledgments This work is supported by the joint DFG/FWF Collaborative Re- search Centre CREATOR (CRC –TRR361/F90) at TU Darmstadt, TU Graz and JKU Linz as well as the Graduate School CE within the Centre for Computational Engineering at TU Darmstadt.

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MULTI-MATERIAL TOPOLOGY OPTIMIZATION OF A ROTATING ELECTRIC MACHINE WITH MECHANICAL CONSTRAINTS

Peter Gangl and **Nepomuk Krenn**

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We consider the topology optimization of a rotating permanent magnet synchronous machine (PMSM) in magnetostatic operation in two space dimensions. We allow a fixed number of possible magnet orientations and ensure stability by imposing mechanical constraints using an augmented Lagrangian approach. This amounts to a multi-material topology optimization problem subject to a system of PDE constraints, coming from nonlinear magnetostatics and linear elasticity.

Following the concept of [1] we represent the design by a vector-valued level set function and update it by the topological derivative taking into account all possible material changes. We derive the topological derivative formulas using a Lagrangian approach [2] which results in the solution of an auxiliary exterior problem and present an efficient way for their numerical computation.

Acknowledgments The authors are grateful for the support of the Austrian Science Fund (FWF) grant F9008.

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HOW TO GAUGE MAGNETOSTATICS TO FACILITATE DOMAIN DECOMPOSITION METHODS

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Low-frequency simulations of electrical machines are crucial for optimizing prototypes with regard to peak performance and minimal energy consumption. Full 3D models are preferable to guarantee accuracy but efficiency suffers due to an increase in computational work compared to the typical 2D simulation. Domain decomposition methods circumvent this problem because they enable the parallel treatment of smaller subsystems from which a global solution can be recovered.

Usually, in low-frequency electromagnetism, potential formulations are applied which feature operators with nontrivial kernels. Hence, there remains an additional challenge concerning the well-posedness of both, the original problem and the local subsystems stemming from the domain decomposition setting. Gauging techniques can be employed to guarantee uniqueness for formulations with or without a decomposed domain.

In this context, we present two different algorithms for solving and gauging the linear system, arising from the typical multiplier-based domain decomposition (FETI [1], Mortaring [2]), in parallel. Furthermore, both methods are examined and compared with a focus on efficiency and speed-up.

Acknowledgments This work is supported by the joint DFG/FWF Collaborative Research Centre CREATOR (CRC – TRR361/F90) at TU Darmstadt, TU Graz and JKU Linz and the Graduate School CE within the Centre for Computational Engineering at Technische Universität Darmstadt.

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ANISOTROPIC MATERIAL LAWS IN NONLINEAR MAGNETOSTATICS

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In magnetostatics the relation between the magnetic field H and the magnetic flux B has to be provided. This relation usually nonlinear and often also anisotropic. The material law is typically given by a function f describing $H = f(B)$. From a physical point of view, f is the derivative of a convex energy density g. The material law is then given by $H = g'(x)$. This is also helpful when applying Newton' s method to the nonlinear system arising after discretization. Convexity of the energy density ensures that basic line search techniques work reliably. In this work we discuss how to fit the energy density g to data and ensure that it can, by construction, only result in a convex function. We present a method for fitting the energy density g based on classical measurement data. Moreover, we illustrate the direct application of this model in finite element simulations, and compare to existing models [1,2], for anisotropic material.

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MULTIPHYSICS SIMULATION OF AN ELECTRIC UPSETTING PROCESS BASED ON LAGRANGIAN FORMULATIONS

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The aim of this work is to describe the mathematical models and numerical methods developed to simulate the electric upsetting process used by the company CIE Galfor in the manufacture of automotive parts, with special attention to electromagnetic phenomena. Electric upsetting is a multiphysics process involving large deformations and fast changes in temperature due to the electric heat generated in the workpiece, made of a ferromagnetic steel whose electromagnetic properties are non-linear and temperature-dependent. The electromagnetic boundary includes electric ports, with known current intensity or voltage drop, involving the use of Lagrange multipliers to set the conditions. The thermo-electromagnetic-mechanical model is described with Lagrangian formulations, well-known for structural models but unusual for coupled electromagnetic-mechanical cases (see, e.g., [1],[2]). To attain this goal, the Eulerian formulation of the eddy current model is presented and then the Lagrangian formulation is deduced by using tools from Continum Mechanics. The 3D formulation is first established and then particularized to the axisymmetric domain of the electric upsetting problem, allowing us to restrict the electromagnetic calculation to the conducting domain. Lastly, some academic tests are shown to validate the results corresponding to the electromagnetic model and the electric-upsetting process.

Acknowledgments The research has been developed in collaboration with CIE Galfor through a project granted by the Centre for the Development of Industrial Technology (CDTI) and signed between the company CIE Galfor and Itmati (nowadays, integrated in CITMAga). This work has been partially supported by Xunta de Galicia under grant 2021 GRC GI-1563 ED431C 2021/15 and MCIN/AEI/10.13039/501100011033/ FEDER Una manera de hacer Europa, under the research project PID2021-122625OB-I00.

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DIRECT SIMULATION OF CHARGE TRANSPORT IN GRAPHENE FET

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A graphene field-effect transistor (GFET) is simulated by direct numerical integration of the Boltzmann transport equation coupled with the Poisson equation for the electrostatic potential. A discontinuous Galerkin method has been adopted for the Boltzmann equation while a finite differences scheme has been used for the Poisson equation [1,2]. The numerical results have been compared with the ones obtained by the drift-diffusion model [3,4]. The findings are useful for the validation of the drift-diffusion and hydrodynamic models for charge transport in semiconductor devices where the active area is made of graphene. As a further extension, the same approach can be used for graphene nanoribbons, bilayer, and multi-layer graphene.

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ANALYSIS AND STABILIZATION OF THE FOIL WINDING MODEL

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Field-circuit coupled problems modeled by the Modified Nodal Analysis lead to systems of differential algebraic equations (DAEs). Numerical treatment of DAEs is more complicated compared to systems of ordinary differential equations because of e.g. the required consistent initial conditions, and the possible sensitivity towards small perturbations. Several index concepts exist to quantify the complexity of DAEs, of which our analysis concentrates on the differentiation index.

In this talk, we present the analysis of the system of DAEs arising from the foil winding model [1]. This complements previous works that have analyzed the field-circuit coupled solid and stranded conductor models [2]. We propose a modified model which stabilizes the foil winding model when high-frequency perturbations are present in the simulation. The stabilized model is shown to be an inductance-like element in the classification of generalized circuit elements [3].

Acknowledgments This work is supported by the German Science Foundation (DFG project 436819664) and the Graduate School CE within the Centre for Computational Engineering at Technische Universität Darmstadt.

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A MIXED FEM FOR THE NONLINEAR MAGNETOSTATIC PROBLEM

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We discuss numerical methods for solving nonlinear magnetostatic problems in two dimensions, which are of relevance in the simulation of electric machines. In contrast to standard approaches, the magnetic flux B is approximated by $H(\mathrm{div})$-conforming finite elements. The discretization thus leads to saddle-point systems, which we reduce to elliptic problems employing hybridization. In this setting, the Lagrange multipliers appearing in this setting correspond to the tangential component of the magnetic field intensity H. As a consequence, both traces $B\cdot n$ and $H\times n$ are available at element interfaces and can be used, e.g., for torque computation. We present numerical experiments and comparisons to existing methods.

A WEIGHTED HYBRIDIZABLE DISCONTINUOUS GALERKIN METHOD FOR DRIFT-DIFFUSION PROBLEMS

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In this talk, I will present a weighted hybridizable discontinuous Galerkin method (W-HDG) for drift-diffusion problems that uses specific exponential weights to eliminate the drift term from local matrix contributions. The proposed scheme is well-posed and exhibits optimal convergence and superconvergence of postprocessed solutions. For polynomial degree zero, dimension one, and vanishing HDG stabilization parameter, W-HDG coincides with the Scharfetter-Gummel finite volume scheme. The use of local exponential weights generalizes the Scharfetter-Gummel scheme to arbitrary high-order approximations, making it a state-of-the-art option for finite volume discretization of transport-dominated problems.

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COUPLED SYSTEMS OF SDES AND SPDES WITH ALGEBRAIC CONSTRAINTS

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This talk is about a new stochastic framework for solving systems arising in circuit simulation. The transient behavior of such networks can be described by systems of partial differential equations coupled via algebraic constraints. We study these systems with uncertainties added by noise sources in the system and on the boundary, e.g. thermal fluctuations. Here, we examine an approach using the semi-explicit prototype

$$\begin{aligned} \mathrm{d}x(t) + f(t,x,y,z,[\omega])\mathrm{d}t - R(t,x,y,z,[\omega])\mathrm{d}W_t^R &= 0, && \text{(SDE)}\\ g(t,x,y,z,[\omega]) &= 0, && \text{(AE)}\\ \mathrm{d}z(t) - A(t,x,y,z,[\omega])\mathrm{d}t - B(t,x,y,z,[\omega])\mathrm{d}W_t^B &= 0 && \text{(SPDE)} \end{aligned}$$

for the coupling of algebraic equations (AE) with a stochastic differential equation (SDE) and a stochastic partial differential equation (SPDE).

We take a look at existing theory and extend this to our prototype to get existence and uniqueness under specific assumptions. Considering these systems, we discuss how restrictive these assumptions are by taking a closer look at circuit simulation in this stochastic setting and see some first numerical results.

HEAT TRANSFER AT NANOSCALE AND BOUNDARY CONDITIONS

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A model of nonlocal heat transfer at nanoscale in rigid bodies is considered. Depending on the relevance of the particular interaction's mechanism between the heat carriers and the lateral walls, three different strategies for the setting-up of the boundary conditions are analyzed, and the consequent forms of the basic fields have been obtained, as well. From the physical point of view, the possible influence of those interactions on the field variables is pointed out. From the mathematical point of view, instead, the well-posedness of the problem is shown [1].

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CUDA PORT TO GPU OF A BOLTZMANN-SCHRÖDINGER-POISSON SOLVER FOR CONFINED DEVICES

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In a previous study, Mantas and Vecil describe an efficient and accurate deterministic solver for nanoscale DG MOSFETs through a deterministic Boltzmann-Schrödinger-Poisson model on a hybrid parallel CPU/GPU platform. The time integration of the Boltzmann equations was ported to the GPU using CUDA extensions, but the computation of the system's eigenstates, i.e. the solution of the Schrödinger-Poisson block, was parallelized only using OpenMP. This work fills the gap by describing a port to GPU for the solver of the Schrödinger-Poisson block.

OPTIMIZED QUANTUM DRIFT DIFFUSION MODEL APPLIED TO A RESONANT TUNNELING DIODE

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The purpose of the study is to optimize a Quantum Drift Diffusion model (QDD) by comparing the solutions with those obtained by the Wigner Transport Equation (WTE) [1], in the case of a Resonant Tunneling Diode (RTD) made of GaAs with two barriers potential made of GaAlAs. The QDD model has been numerically solved by using finite difference scheme for Poisson equation and Scharfetter-Gummel scheme for continuity equation, in the stationary case. To solve the WTE we have adopted a signed Monte Carlo method [2]. To optimize the QDD model we have used a constrained optimization procedure.

A good agreement between the two models is found when the applied bias voltage is low. Furthermore, we have compared the QDD model with a Quantum Hydrodynamical model [3], solved by using a Runge-Kutta Discontinuos Galerkin method.

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MS 22

Organizers: Poul G Hjorth, Agnieszka Wyłomańska, Janusz Szwabiński, Hilary Ockendon, Kamil Kulesza

Abstract The purpose of these four talks is to give an overview of the breadth of applicability of industrial mathematics and the breadth of mathematical imagination that this may entail.

	Thursday
Room	CR 10 AC
17:20-17:45	John and Hilary Ockendon
17:45-18:10	Agnieszka Wyłomańska
18:10-18:35	Kamil Kulesza
18:35-19:00	Janusz Szwabiński

THE ESSENCE OF MATHS IN INDUSTRY

Hilary Ockendon[a] and **John Ockendon**[a]

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The expression Maths in Industry has only been in common use for the past 50 years but throughout that short time it has embraced an ever increasing range of scientific activity. This has involved all of applied maths, including computation and statistics as well as most branches of physical, biological, social and economic science. It has been at its most successful when the collaboration has involved

1. Sympathy from industrial participants;
2. The industrial challenge can be framed as a well-defined mathematical model;
3. The challenge is addressed by open minded and imaginative mathematicians;
4. The outcome is of value to industry and
5. The outcome opens up new lines of mathematical research.

This presentation will discuss these 5 aspects in more detail and illustrate them with examples from a wide variety of industries and involving a wide range of mathematical techniques.

ACADEMICS WORKING IN THE MARKET ENVIRONMENT

Kamil Kulesza

Long-running discussion on how to finance industrial maths academic activities is crucial to the essence of maths in industry.

Among the reasons why it is so important is that running projects with partners from industry gives a vital feedback loop that allows us to judge the value of a project. This is especially true if the industrial partner finances the project.

The other important aspect is gaining resources for mathematical research that is orthogonal to the traditional grant mechanisms and results in much greater independence. Nonetheless, it seems that public money has its role to play, for instance in the form of seed money to foster new industrial maths activities or for training of the next generations of researchers. In my talk I want to raise three points that seem to be crucial when doing industrial maths in the market environment. My message draws from almost 20 years of experience in such operations, all in the self-financing regime outlined below. As such the message might be useful for both seasoned academics running industrial maths operations, as well young cohorts, especially graduate students and postdocs.

The following points will be discussed:

1. Interdisciplinary and even multidisciplinary teams are of great value - do not restrict teams' members to mathematicians or seasoned people alone. [motto: "Probabilistic Logic and the Synthesis of Reliable Organisms from Unreliable Components" –John von Neumann (the title of seminal paper)]
2. Problems –industrial relevance and mathematical novelty [motto: "The challenge is to join, in one body, academic creativity and military efficiency of execution" –Andy Hopper, FRS, one of computer science icons and serial entrepreneur]
3. Involving decision-making executives [motto: "I have a system" –Andy Hopper's frequent answer to various questions of a type 'how did you manage to do it?']

TOWARDS A NANOPARTICLE BASED DRUG DELIVERY SYSTEM: INSIGHTS FROM SINGLE PARTICLE TRACKING DATA

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In order to design efficient nano delivery systems for drugs and genes, at least partial understanding of the mechano-structural characteristics of living matter is crucial. The nanoparticle carriers of drugs for instance often must overcome diverse biological barriers in order to achieve therapeutic efficacy in target cells, tissues and organs. Hence, quantitative models revealing the microscopic structure and rheology of biological specimens are needed.

In recent years, single particle tracking (SPT) has become a popular method to quantify the motion of individual particles in living matter at high spatial and temporal resolution. In a typical SPT measurement the molecules of interest are tagged with fluorescent dye particles. After illumination by a laser, the labels produce light and their positions may be determined with a microscope. Using lasers that flash at short time intervals allows for tracking of the movement of the molecules over time. The recorded positions are used to reconstruct trajectories of individual molecules. These trajectories are then analyzed in order to extract local physical properties of the molecules and their environment, such as velocity, diffusion coefficient (or tensor), and confinement (local density of obstacles).

The analysis of SPT trajectories is not a trivial task due to the stochastic nature of the molecules' movement. It usually starts with the detection of a corresponding motion type of a molecule, because this information may already provide insight into mechanical properties of its surroundings. In this talk, several methods for identification of the motion types will be presented, starting with the very popular technique based on mean-square displacement of particles, through statistical hypothesis testing and feature-based machine learning, ending up with the deep learning classification methods.

DOES THE INDUSTRY NEED MATH?

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A number of examples show that today's industry needs advanced mathematical methods. Based on long-time experience and many years of cooperation with the industry (especially mining industry), it will be shown that seemingly unrelated disciplines (such as mining and mathematics) have a chance to work together, and, moreover, it gives benefits to both sides. On the one hand, the mining industry needs more and more advanced techniques to describe the processes observed in the mines. An example might be methods to detect anomalies in the operating parameters of mining machinery. Without advanced apparatus and modern algorithms, early detection of defects in such machines is not possible. On the other hand, real problems observed in industry become the basis for proposals for new mathematical methods and new theories. The presentation will show examples of the use of mathematical methods for the detection of local damage in mining machines, as well as examples of new mathematical theories that arise from real problems in the mining industry.

MS 23

Organizers: Marek Teuerle, Christophe Picard

Abstract Due to the era of digitization in learning environments that was recently boosted by the COVID-19 pandemic, we observe new challenges in the field of education. This minisymposium, hosted by the ECMI Educational Committee, presents the educational experience in applied and industrial mathematics among various centers of the ECMI network and their partners. It also includes a discussion panel about the Data Science Model Master, which is a running project by the ECMI Educational Committee.

	Wednesday
Room	CR 10B
10:40-12:20	Chairperson: M. Teuerle
10:40-11:05	Danijela Rajter-Ćirić
11:05-11:30	Ewald H. Lindner
11:55-12:20	Markus Grasmair
11:55-12:20	Martin Bracke
15:30-16:45	Chairperson: Ch. Picard
15:30-15:55	Lukas Bayer
15:55-16:20	Danijela Rajter-Ćirić
16:20-16:45	Marek Teuerle

DIGITAL LEARNING ENVIRONMENTS DURING COVID-19 PANDEMIC

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During the Covid-19 pandemic, the implementation of many of our traditional event formats for interdisciplinary STEM projects with students was not possible. Like many others, we then developed alternative materials and looked for opportunities for hybrid or purely virtual formats.

In this talk, we would like to present examples of digital learning environments on the topics of "Mathematical Models for Disease Propagation" as well as "Evacuation Scenarios" (see [1]), which we have since made available to schools for use. We have also used the material in our own practical courses for students and can give an experience report.

In this context, we would also like to give a summary of our experiences with digital and hybrid forms of teaching and learning and our conclusions from the pandemic.

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MODELING WEEKS AND STEM PROJECTS IN HIGH AND MIDDLE SCHOOLS

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Mathematical modeling weeks for students have a long tradition in Kaiserslautern and have taken place up to four times a year since their introduction in 1993. From this, the more compact event form of modeling days has developed, which is regularly held with entire classes in different schools. This also involves teachers, who also have the opportunity to earn a STEM certificate based on several modules.

Another variant are the so-called Junior Engineer Academies, each of which works on a major STEM project for a total of three years in middle school. As a short format, we conduct workshops for gifted students, for some time now also in the very popular subject area „AI and Machine Learning “, which is illuminated and experienced from a mathematical perspective.

In this talk, we present the different formats with examples of content and our practical experience as well as outlooks on future developments.

THE ETHIOPIAN-NORWEGIAN NETWORK IN COMPUTATIONAL MATHEMATICS

Markus Grasmair[a], **Anne Kværnø**[a] and **Zerihun Kinfe Birhanu**[b]

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Since 2007, Hawassa University, Ethiopia, and NTNU, Norway, have been building up first a master programme and then a PhD programme in applied mathematics and statistics at Hawassa University. Moreover, we have recently received funding for a course development and exchange programme that includes two additional Ethiopian universities (Adama and Arba Minch). In particular, this programme allows us to organise Ethiopian modelling weeks, study groups with industry, as well as winter schools on topics relevant for industrial mathematics. In this talk, we will present our experiences from the previous and current projects as well as our ambitions for the future.

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20 YEARS MASTER PROGRAMME "INDUSTRIAL MATHEMATICS" AT JKU LINZ

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By October 1, 2003 JKU Linz switched from the former diploma programme "Technical Mathematics" to the Bologna scheme with one bachelor and three master programmes. We will present the master programme "Industrial Mathematics" and its modifications sincce 2003, the cooperation with Eindhoven University of Technology and the Technical University Kaiserlautern (now RPTU) with respect to the Double Degree Programme in "Industrial Mathematics" and the impact of Covid-19 for teaching at JKU Linz (3G-, 2.5G-, 2G-rules, lockdowns and re-openings).

CHALLENGES OF ONLINE TEACHING OF APPLIED MATHEMATICS COURSES

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We are living in a digital world, and today many processes are done or can be done virtually. Teaching is one of the processes that has undergone great transformations regarding that matter, especially in the last years. At the Department of Mathematics and Informatics at Faculty of Sciences in Novi Sad there have been study programs of Applied Mathematics that abound in a large number of professional subjects in the field of Data Science or Artificial Intelligence. From the very beginning it has been a challenge to organize classes for such subjects. During the pandemic, almost all teaching was done online and it was a challenge for teachers to organize their lectures in such a way as to enable students to acquire skills as planned in the syllabus and at the same time to maintain essential parts of the teaching process. Advanced online classroom software has a very important role, but the most important role is the one that teachers have. The possible ways of online teaching of Applied Mathematics courses and challenges that teachers and students are facing during the virtual realization of such lectures are topics we will focus on during this talk.

DATA SCIENCE MASTER STUDY PROGRAM AT FACULTY OF SCIENCES IN NOVI SAD

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The master study program *Applied mathematics - Data Science* was introduced at Department of Mathematics and Informatics at Faculty of Sciences in Novi Sad in 2016 and since the beginning it attracts many students. The goal of the study program is the education of mathematicians in the field of Applied Mathematics, especially Data Science, as experts in the economy, industry (especially in information and communication technologies), medicine, economic and financial institutions. Through teaching content, the study program ensures the improvement of fundamental knowledge acquired at the previous level of schooling, the acquisition of knowledge and competition for work in the field of data analysis, but also the continuation of education in doctoral studies in mathematics or IT, depending on the chosen module. Modernization of the curriculum is regularly carried out by harmonizing the subject content with modern trends in the scientific field to which the subject belongs. Also, there is a possibility of introducing new optional subjects if the need arises. During this talk we will present the curriculum and we will also discuss some crucial aspects of the study program.

DISCUSSION ABOUT THE ECMI DATA SCIENCE MODEL MASTER

Moderator: Marek Teuerle

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Recently, ECMI Educational Committee [1] started discussion on ECMI Data Science Model Master, which similarly to ECMI Technomathematics and Economathematics Model Master structures [2], will be a guideline among ECMI members and prospective candidates to establish an ECMI certified master programme in the areas of Data Science/Big Data/Data Engineering. During this panel, we will present the current development of the project and later have a discussion on this topic.

References

1. https://ecmiindmath.org/bodies-of-ecmi/educational-committee/
2. https://ecmiindmath.org/education/ecmi-model-master-in-mathematics-for-industry/

MS 24

Organizers: Milene Santos and Ricardo Costa

Abstract Differential equations have an essential role in the mathematical modelling of real-world applications across several fields such as engineering, biomedicine, and socio-economic sciences. In that regard, the ever-increasing complexity of these applications has raised important challenges in the quest for accurate and efficient numerical methods: How to preserve accuracy with boundary conditions prescribed on arbitrary curved boundaries without relying on curved meshes? How to achieve larger time-steps in stable time discretisations without accuracy deterioration? These are some of the questions numerical scientists seek to solve, and alternative schemes to the classical approaches have been recently proposed to achieve optimal order of convergence. This mini-symposium aims to cover some of the most recent advances in numerical methods for solving differential equations with high-order convergence and efficiency.

	Friday
Room	CR 113
10:40-11:05	Ricardo Costa
11:05-11:30	Milene Santos
11:30-11:55	Gaspar J. Machado
11:55-12:20	Jacek Miękisz

VERY HIGH-ORDER ACCURATE FINITE VOLUME SCHEMES ON POLYGONAL MESHES FOR CURVED BOUNDARY PROBLEMS

Ricardo Costa[a], **Stéphane Clain**[b], **Gaspar J. Machado**[c], **João M. Nóbrega**[a] **Hugo Beirão da Veiga**[d] and **Francesca Crispo**[e]

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Real-world problems in physics and engineering often involve complex curved geometries. The numerical solution of differential equations in such domains raises challenging numerical issues in developing accurate and robust discretisation techniques, particularly in the context of very high-order accurate methods. In that regard, the conventional treatment of curved boundaries relies on curved meshes to eliminate the geometrical mismatch between the physical and computational boundaries and recover the optimal convergence orders. However, sophisticated meshing algorithms, cumbersome quadrature rules on curved elements, and complex non-linear transformations are necessary. Significant advances have been recently achieved towards alternative discretisation techniques that solely use polygonal meshes with a linear piecewise approximation to the curved physical boundary. The present work proposes a novel approach, the reconstruction for off-site data method [1,2], employed within the finite volume method to discretise relevant problems in physics and engineering. The technique imposes general boundary conditions via polynomial reconstructions with specific linear constraints defined for a set of points on the physical boundary, and the numerical fluxes are computed on the polygonal mesh elements. Several benchmark test cases of fluid flow problems in three-dimensional arbitrary curved domains confirm that the proposed method effectively achieves very high-orders of convergence.

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COMPACT SCHEMES IN TIME WITH APPLICATIONS TO PARTIAL DIFFERENTIAL EQUATIONS

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Following [1], we propose a new class of fourth- and sixth-order schemes in time for parabolic and hyperbolic equations. The method follows the compact scheme methodology by elaborating implicit relations between the approximations of the function and its derivatives. Several benchmarks for Ordinary Differential Equations demonstrate the effectiveness of the method. Then a second set of numerical benchmarks for Partial Differential Equations such as convection-diffusion, Schrödinger equation, wave equation, Bürgers, and Euler system give the numerical evidence of the stability of the schemes and the achievement of the optimal orders of convergence.

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M.T. Malheiro acknowledges the financial support by Portuguese Funds through Foundation for Science and Technology (FCT) in the framework of the Projects UIDB/00013/2020 and UIDP/00013/2020 of CMAT-UM.
S. Clain, G.J. Machado, and M.T. Malheiro acknowledge the financial support by FEDER – Fundo Europeu de Desenvolvimento Regional, through COMPETE 2020 – Programa Operacional Fatores de Competitividade, and the National Funds through FCT, project no. POCI-01-0145-FEDER-028118.

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EVOLUTIONARY GAMES WITH STRATEGY-DEPENDENT TIME DELAYS

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It is well known that time delays can cause oscillations in dynamical systems. Usually, the internal equilibria of evolving populations, describing the coexistence of strategies, are expected to be asymptotically stable for small time delays, while above the critical time delay at which the Hopf bifurcation occurs, they become unstable, cycles appear. Here we present a new behavior of systems with time delays, not present in any previous models of evolutionary games [1]. We show that in differential replicator equations with strategy-dependent time delays, interior stationary states, describing the level of cooperation in evolutionary games of social dilemmas, depend continuously on time delays. We also show that they may disappear or additional states can emerge.

In the Prisoner's Dilemma game, for time delays of cooperation smaller than ones of defection, an unstable interior state appears, so for some initial conditions, the population converges to a homogeneous state with just cooperators.

We will also discuss some results for finite populations, preliminary ones were presented in [2].

Acknowledgments This project has received funding from the European Union' s Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 955708.

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VERY HIGH-ORDER ACCURATE DISCONTINUOUS GALERKIN METHOD FOR CURVED BOUNDARIES WITH POLYGONAL MESHES

Milene Santos[a], **Adérito Araújo**[a], **Sílvia Barbeiro**[a], **Stéphane Clain**[a], **Ricardo Costa**[b,c] and **Gaspar J. Machado**[d,e]

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Preserving the optimal convergence order of discontinuous Galerkin (DG) discretisations in curved domains is a critical and well-known issue [1]. The proposed approach relies on the reconstruction for off-site data (ROD) method developed originally within the finite volume framework [2]. The main advantages are simplicity, since only piecewise linear boundary approximations are used, and versatility, since any type of boundary condition can be imposed. The developed DG–ROD method consists in splitting the boundary conditions treatment and the leading discrete equations from a classical DG formulation into two independent solvers coupled in a simple and efficient iterative procedure. A numerical benchmark is provided to assess the capability of the method with Dirichlet and Neumann boundary conditions prescribed on curved boundaries, demonstrating that the optimal convergence order is effectively achieved.

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MS 25

Organizers: Krzysztof Burnecki, Joseph Klafter, Marcin Magdziarz, Aleksander Weron

Abstract Three Nobel Prizes awarded within a short five year period (2009 in Physiology or Medicine, 2012 and 2014 in Chemistry) were related to the biological mechanisms in living cells and the fluorescence-based techniques of observing these mechanisms under the microscope. The accessibility of quantitative data prompted many physicists and applied mathematicians to study single biological cells and the physiological processes running off therein. During the minisymposium (i) advancements of the mathematical theory of (transient) anomalous diffusion, (ii) rigorous statistical inference methods tailored for single particle tracking data, and (iii) techniques for identification, validation and prediction of anomalous dynamics in living cells will be presented.

	Wednesday
Room	CR 10 AC
11:30-12:20	Chairperson: Marcin Magdziarz
11:30-11:55	Yuval Garini
11:55-12:20	Ralf Metzler
11:20-13:00	Chairperson: Joseph Klafter
15:30-15:55	Diego Krapf
15:55-16:20	Kacper Taźbierski
16:20-16:45	Monika Muszkieta
16:45-17:10	Jakub Ślęzak

	Friday
Room	CR 114
10:40-12:20	Chairperson: Aleksander Weron
10:40-11:05	Aleksei Chechkin
11:05-11:30	Michał Balcerek
11:30-11:55	Marek Teuerle
11:55-12:20	Joanna Janczura

DOUBLY STOCHASTIC FRACTIONAL BROWNIAN MOTION

Michał Balcerek[a], **Krzysztof Burnecki**[a], **Samudrajit Thapa**[d], **Ralf Metzler**[b], **Agnieszka Wyłomańska**[a] and **Aleksei Chechkin**[a,b,c]

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In my talk I will explore the extensions of fractional and multifractional Brownian motion by introducing stochastic modulation of the Hurst parameter or function. This involves generalizing the properties of these processes and developing a method to distinguish between each case. Finally, I will demonstrate the application of this method on real-world data, showcasing the obtained results. The case of randomizing the Hurst parameter in the classical fractional Brownian motion was already investigated in [1], but the need for even more general model is recently mentioned e.g. in [2].

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WHEN SINGLE PARTICLE TRACKING DOES NOT WORK: ANOMALOUS DIFFUSION OF EXCITONS IN NANOMATERIALS

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The diffusion of excitons in perovskites and transition metal dichalcogenides shows clear anomalous, subdiffusive behaviour in experiments. We develop a non-Markovian mobile–immobile model which provides an explanation of this behaviour through paired theoretical and simulation approaches. The simulation model is based on a random walk on a 2D lattice with randomly distributed deep traps such that the trapping time distribution involves slowly decaying power-law asymptotics. The theoretical model uses coupled diffusion and rate equations for free and trapped excitons, respectively, with an integral term responsible for trapping. The model provides a good fitting of the experimental data, thus, showing a way for quantifying the exciton diffusion dynamics.

References

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UNVEILING THE WONDERS OF CELL NUCLEUS DYNAMICS

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The cell nucleus plays a pivotal role in housing our genetic code, and understanding its dynamics is vital for comprehending its function. Extensive research over the past decade has focused on establishing the mathematical foundations that govern this dynamic behavior, continually yielding fresh insights.

I will outline the principal modes of dynamics that we have recently identified, based on single particle tracking methods, and emphasize their significance in relation to cellular function.

IDENTIFYING HETEROGENEOUS DIFFUSION STATES IN THE CYTOPLASM BY A FRACTIONAL BROWNIAN MOTION WITH SWITCHING

Joanna Janczura

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We analyze individual trajectories of quantum dots in the cytoplasm of living cultured cells using a hidden Markov model with volatility switching. Based on the expectation-maximization algorithm we identify two distinct mobility states with an overall sub-diffusive mode of motion of the fractional Brownian motion (FBM) type. Using the extracted features of experimental trajectories as input for simulations of different variants of a two-state FBM model, we show that the trajectory-intrinsic and the ensemble-wise heterogeneity in the experimental data is mostly due to variations in the process parameters. Altogether, our approach shows that diffusion heterogeneities can be faithfully extracted and quantified from fairly short trajectories obtained by single-particle tracking in highly complex media. [1]

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MEASURING AND MODELING HETEROGENEOUS DIFFUSION IN THE CYTOPLASM OF LIVING CELLS

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We study the motion of quantum dots and individual messenger RNA (mRNA) in the cytoplasm of HeLa cells using single-particle tracking. The trajectories are analyzed in terms of the mean squared displacement and the power spectral density. We observe that the motion resembles an antipersistent random walk, which suggests fractional Brownian motion as a useful model. However, the trajectories alternate between different states due to cellular heterogeneities and interactions with specific partners. Quantum dots randomly switch between different mobility states, which can be dissected using a hidden Markov model [1,2]. Our data indicate that one of these states is rooted in the transient associations with the cytoskeleton-shaken endoplasmic reticulum network. In contrast to the quantum dot trajectories, mRNA dynamics exhibit aging and ergodicity breaking. These complexities are found to be governed by heterogeneous interactions where the residence times in a bound state have a heavy-tailed distribution.

Acknowledgments The author acknowledges the support from the National Science Foundation grant 2102832.

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LONG-RANGE CORRELATED PROCESSES: CONFINEMENT & HETEROGENEITY

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Stochastic processes driven by Gaussian yet power-law correlated noise, such as Mandelbrot's fractional Brownian motion (FBM) represent a quite ubiquitous effective description of the dynamics in a range of complex systems, e.g., for the motion of tracers in viscoelastic environments, in "rough" financial data, or for the persistent motion of animals. FBM is an ergodic yet strongly non-Markovian process, with often surprising behaviour. In this talk I will briefly introduce these processes and demonstrate that in strong confinement their probability density may assume non-Boltzmannian, multimodal stationary shapes, while in soft external potentials no steady state exists. An application of this effect to brain fibre growth is discussed. In heterogeneous environments the memory correlations of a diffusing test particle may become a (random or deterministic) function of time or space. For these cases I will introduce "doubly-stochastic" extensions such as FBM with random scaling exponent, memory-multimodal FBM, and FBM with a "diffusing diffusivity".

INTERPOLATION OF FRACTIONAL BROWNIAN TRAJECTORIES FOR A SINGLE PARTICLE TRACKING EXPERIMENT

Monika Muszkieta and **Joanna Janczura**

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In the talk, assuming that particles undergo the fractional Brownian motion, we will introduce the interpolation model based on the fact that the spectral density derived for the finite-length realization of this process obeys a power law decay [1]. This will allow us to apply the main idea of compressed sensing to reconstruct a given trajectory in the frequency domain. We will consider various trajectory degradation models reflecting typical limitations found in a single particle tracking experiment. On the basis of the obtained results of the statistical analysis [2] we will show that parameters characterizing the fractional Brownian motion estimated from trajectories interpolated by the proposed method are close to the ones estimated from the ground truth data.

References

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RANDOM COEFFCIENT AUTOREGRESSIVE PROCESSES AS DIFFUSION MODELS

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Many studies on biological and soft matter systems report the joint presence of a linear mean-squared displacement and a non-Gaussian probability density exhibiting, for instance, exponential or stretched-Gaussian tails. This phenomenon is ascribed to the heterogeneity of the medium and is captured by random parameter models such as "superstatistics" or "diffusing diffusivity". Independently, scientists working in the area of time series analysis and statistics have studied a class of discrete time processes with similar properties, namely, random coefficient autoregressive models. We present how to try to reconcile these two approaches and thus provide abridge between physical stochastic processes and autoregressive models. We start from the basic Langevin equation of motion with time-varying damping or diffusion coefficients and establish the link to random coefficient autoregressive processes. By exploring that link we gain access to efficient statistical methods which can help to identify data exhibiting Brownian yet non-Gaussian diffusion [1].

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SERIES REPRESENTATION OF PROCESSES WITH RENEWAL RESETTING

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Processes with resetting have found applications in e.g. modelling various searching strategies and foraging patterns, where the living organism after an unsuccessful excursion returns to the initial position and start the search again. In the field of population dynamics resetting could be interpreted as a random event reducing population to its natural size according to the environmental capacity.

We introduce a series representation for stochastic processes with resetting guided by a renewal process. There, a process follows the same law on each interval, being determined by successive renewal times. In these points in time the process is being reset to a constant point in space. Both memory-erasing (complete) resetting, where the process starts anew, and simple position shifting (incomplete resetting) are considered.

Our approach allows us to calculate PDFs of the processes, joint PDF at two points in time, autocorrelation function in an intuitive and straightforward manner. We also study the first passage problems, with general results obtained for the case of complete resetting. For each general result we inspect the case for exponentially (Poissonian resetting) and mixture-exponentially distributed interresetting times, with Brownian motion and scaled Brownian motion as the underlying processes. The mixture-exponential distribution allows us to approximate results for other distributions in a manner similar to De Vylder method.

Acknowledgments
This research was partially supported by *Narodowe Centrum Nauki* Sonata Bis-9 grant nr 2019/34/E/ST1/00360.

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LÉVY WALKS AND FRACTIONAL MATERIAL DERIVATIVE - NUMERICAL APPROXIMATIONS

Marek Teuerle, and **Łukasz Płociniczak**

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A Lévy walk process was proposed by Klafter, Blumen and Shlesinger in 1982 [1]. It was introduced as the microscopic description of dynamics within the continuous-time random-walk framework by including tight spatio-temporal coupling between heavy-tailed jumps and waiting times. The model has become a useful tool in modelling various anomalous diffusion processes that are characterised by finite-second moments. Namely, it has been applied in biological systems to describe the spatial collective behaviour of bacteria, bumblebees, seabirds, marine predators and humans, in statistical physics to describe the dynamics of cold atoms, blinking quantum dots, and random search strategies (for other examples, see the comprehensive review: [2]).

Recently, the macroscopic characteristics of Lévy walks have been investigated. In particular, the scaling limits of their behaviour, as observed through Skorokhod's J_1 convergence, were identified as α-stable processes that are subjected to strongly dependent inverse α-stable subordinators. This finding is a consequence of a strong interdependence between waiting times and jumps within the underlying microscopic scenario of the Lévy walk [3]. The results also show that the scaling limits' dynamics is governed by the so-called fractional material derivative [3], [4], which generalises the concept of the classical material derivative to fractional calculus.

In this work, we investigate the problem of numerical approximations of the fractional material derivative. We propose a numerical scheme that is based on spatiotemporal coupling and the known techniques proposed for fractional derivatives [5]. The stability of the scheme is established through rigorous analysis. Moreover, the accuracy of the introduced finite-volume upwind method is verified for the case of a one-sided probability problem related to Lévy walks and compared with the usual Monte Carlo approach.

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MS 26

Organizers: Krzysztof Burnecki, Zbigniew Michna and Marek Teuerle

Abstract In examining the nature of the risk associated with a portfolio of policies in an insurance company, it is often of interest to assess how the portfolio may be expected to perform over an extended period of time. One approach concerns the use of ruin theory. Ruin theory is concerned with the excess of the collected premiums over the claims paid. Moreover, if we consider an insurance company with different lines of business related to various perils or an insurance company with its reinsurers, the risk model becomes multidimensional. We will consider here different mathematical aspects of the ruin probability in finite and infinite time and other risk assessment tools in the context of insurance, reinsurance companies and pension funds.

	Tuesday
Room	CR 113
17:20-17:45	Audrius Kabašinskas
17:45-18:10	Krzysztof Kępczyński
18:10-18:35	Zbigniew Michna
18:35-19:00	Aleksandra Wilkowska

ON SYSTEMIC RISK ASSESSMENT OF LITHUANIAN SECOND-PILLAR PENSION FUNDS

Audrius Kabašinskas

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Pension funds are an essential part of retirement planning, and their performance and risks play a significant role in ensuring financial stability for retirees. This study aims to analyse the connectedness and spillover effects in the Lithuanian second-pillar pension fund market. The findings of this study provide insight on the interdependence within the second-pillar pension funds market and with other financial markets, and contribute to a better understanding of the risk-return trade-off of pension funds, especially during high-volatility periods. Differently from other studies in this paper market regimes are identified using hidden Markov models. Interdependence (including multivariate and non-linear) and causality between pension funds are analysed in different market regimes. Finally, returns spillover in different regimes is estimated using VAR and VECM models. The results of this paper are expected to be useful for pension fund managers, participants, and pension system supervisors in making decisions about investment strategies and in practices of systemic risk management regulation.

This project has received funding from the Research Council of Lithuania (LMTLT), agreement No S-MIP-21-32.

PROPORTIONAL REINSURANCE FOR BROWNIAN RISK MODEL

Krzysztof Kępczyński

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This talk investigates ruin probabilities for a two-dimensional Brownian risk model with drift dependant initial capital. We focus on simultaneous ruin probabilities in a finite-time horizon. We derive the asymptotics as the initial capital and drift tend to infinity.

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SIMULTANEOUS RUIN PROBABILITY FOR TWO-DIMENSIONAL BROWNIAN AND LÉVY RISK MODELS

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The ruin probability in the classical Brownian risk model can be explicitly calculated for both finite and infinite-time horizon. This is not the case for the simultaneous ruin probability in two-dimensional Brownian risk model. Resorting on asymptotic theory, we derive approximations of both simultaneous ruin probability and simultaneous ruin time for the two-dimensional Brownian risk model when the initial capital increases to infinity. Moreover given the interest in proportional reinsurance, we consider in some details the case where two insurance companies (or two branches of the same company) divide between them both claims and premia in some specified proportions. This model is tractable allowing for explicit formulas of the simultaneous ruin probability for spectrally asymmetric Lévy processes. Examples include Brownian motion, α-stable Lévy processes, gamma process and perturbed gamma process.

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PROBABILITY OF RUIN IN THE MODEL OF COLLABORATING INSURANCE COMPANIES

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In this talk we will discuss the problem of ruin probability for a two-dimensional insurer-reinsurer risk process. A proportional reinsurance model applies to a situation where claims are divided according to a predetermined proportion between two insurance companies (the insurer and the reinsurer). We will present two explicit formulas for determining the probability of ruin and two practical universal approximations. The first explicit formula ([3]) relates to the case where the claims are from an exponential distribution. The second applies to the case when the claims are described by a phase-type distribution ([4]) for which there are real solutions of the Lundberg equation. The first of the proposed approximations is based on De Vylder's idea ([1]), while the second one is based on the concept of diffusion approximation ([2]). The accuracy of the results is analyzed numerically and we will perform results of the analysis, which confirms satisfactory accuracy of obtained results.

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Part VI

Contributed talks

CT 01

	Monday
Room	CR 113
17:20-17:45	Rafael Henriques
17:45-18:10	Halvor Snersrud Gustad

A HYBRID MODEL FOR PREDICTING BENDING MOMENTS IN SUBSEA STRUCTURES USING MOTION SENSORS AND RNNs

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Subsea structures in offshore petroleum operations are subject to significant fatigue due to operation conditions and environmental loads. Predicting bending moments at exposed positions near flex joints is essential for maintenance scheduling and reducing downtime. In this talk we present a method for predicting bending moments at exposed positions near the flex joint using only motion sensors. We use Recurrent Neural Networks (RNNs) combined with a mathematical model of the flex joint to create a system able to predict bending moments to an acceptable level of accuracy. Specifically, we train the RNN to learn the underlying dynamics of the flex joint using data from the motion sensors.

The RNN model is based on the assumption that it is a discretization of an underlying dynamical system. An analysis of the recurrent neural network is provided along with propositions for improved discretization methods. By using the hybrid model we can provide a valuable resource helping the user preform a safer and more efficient operation.

THE FINITE ELEMENT METHOD WITH NEURAL NETWORKS TO RECONSTRUCT THE MECHANICAL PROPERTIES OF AN ELASTIC MEDIUM

Rafael Henriques and **Sílvia Barbeiro**

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In this work we investigate a mathematical model to reconstruct the mechanical properties of an elastic medium, for the optical coherence elastography imaging modality. To this end, we propose machine learning tools by exploring neural networks to solve the inverse problem of elastography. In our framework, we analyze the relative error between the exact function and the neural network for the case of noise free data and noisy data. The direct problem is used to define the cost function. Our algorithm updates the parameters combining the backpropagation technique with the ADAM optimizer to minimize a cost function that takes into account the error of using neural networks in the fully discretized scheme of the direct problem. We report several computational results using fabricated data with and without noise.

Acknowledgments This work was supported by FEDER Funds through the Operational Program for Competitiveness Factors - COMPETE and by Portuguese National Funds through FCT - Foundation for Science and Technology "2021.06672.BD" and the Centre for Mathematics of the University of Coimbra - UIDB/00324/2020, funded by the Portuguese Government through FCT/MCTES.

CT 02

	Monday
Room	CR 115
15:30-15:55	Leon Baeck
15:55-16:20	Thi Thai Le
16:20-16:45	Merab Svanadze
16:45-17:10	Emma Greenbank

TOPOLOGY OPTIMIZATION OF A BIPOLAR PLATE

Leon Baeck[a], **Sebastian Blauth**[a], **René Pinnau**[b] and **Kevin Sturm**[c]

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Hydrogen technologies are set to play a major role in the process of achieving climate-neutral mobility and a clean energy industry. In this context, the production of hydrogen with electrolysis cells is of high importance. Here, water is split into hydrogen and oxygen using (green) electrical energy. Essential for the performance of a PEM electrolysis cell are the flow dynamics of the so-called bipolar plates.

In this talk, we consider the topology optimization for the anode side bipolar plate of a PEM electrolysis cell by using the topological derivative. The goal of the optimization is to achieve a uniform flow distribution throughout the plate by taking aspects of manufacturability into account. Our approach gives rise to novel designs that could be used to improve the performance of PEM electrolysis cells.

HOMOGENISATION AND MODELLING OF A SILICON NANOWIRE LI-ION BATTERY ANODE

Emma Greenbank, **Doireann O'Kiely** and **Michael Vynnycky**

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The use of silicon in lithium ion batteries poses some major challenges in battery design. One major challenge is the extreme volumetric change of silicon during lithiation in the normal operation of the battery. The stresses resulting from this swelling can cause degradation and failure of the battery. This talk focuses on an anode design introduced in 2019 to alleviate these issues. The anode is composed of an array of copper nanowires, coated with Li-carrying copper silicide and surrounded by Li-alloying electrolyte [1], [4]. The focus of this work is twofold. Firstly, the homogenisation of the anode using techniques from Hunt *at el.* [3] and Moyles *at el.* [2]. Secondly, numerical solutions of the homogenised problem are used to predict the transport of lithium through the anode. We will assess the accuracy and implications of these predictions, and outline plans for further modelling.

Acknowledgments This research was supported in part by a grant from Science Foundation Ireland under Grant number 12/RC/2289-P2.

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KELVIN-HELMHOLTZ INSTABILITY'S ROLE IN ENERGY TRANSITION PROCESSES

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The ongoing energy transition demands sustainable and efficient energy storage, production, and consumption. In this context, the role of the Kelvin-Helmholtz instability in enhancing the efficiency of energy transition processes is critical. The instability arises from fluid flow interaction with different velocities, resulting in complex flow patterns that can significantly affect efficiency and performance. The Kelvin-Helmholtz instability can occur in various renewable energy technologies, such as wind turbines and tidal energy converters, reducing efficiency and increasing maintenance costs. In wind turbines, the instability can occur in the boundary layer between the atmosphere and the blades, generating turbulent flow that reduces efficiency. Similarly, in tidal energy converters, the instability can cause a fluctuating flow pattern that reduces the turbine's efficiency and increases blade wear and tear. In this talk, we will explore the Kelvin-Helmholtz instability's impact on energy storage challenges, specifically during the injection and withdrawal of gases, such as hydrogen and natural gas, into underground storage [1]. The instability arises from the co-existence of different gases. Besides this, the geometric factors, such as the storage reservoir's shape and size or the media's porosity and permeability [2], can influence the onset and development of the Kelvin-Helmholtz instability, affecting the storage process's efficiency, including the injection and withdrawal rate. Finally, we will highlight the potential of the Kelvin-Helmholtz's instability to support a sustainable and efficient energy transition.

Acknowledgments This work has been conducted in the EnergyLab of the Research Campus MODAL funded by the German Federal Ministry of Education and Research (BMBF) (fund numbers 05M14ZAM, 05M20ZBM).

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ON THE COUPLED THEORY OF THERMOELASTICITY OF NANOPOROUS MATERIALS

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Prediction of mechanical properties of nanoporous materials is one of the current topics of continuum mechanics. Many of the engineering problems have coupled physical nature, and it is required to consider several coupled mechanical concepts simultaneously in the models of such materials. Recently, Svanadze [1,2,3,4] introduced the linear models of elasticity and thermoelasticity for materials with single and double porosity in which the coupled phenomenon of the concepts of Darcy' s law and the volume fraction of pore network is considered. In this work, the 3D linear coupled mathematical model of thermoelasticity for nanomaterials with triple porosity is presented in which the coupled phenomenon of the concepts of Darcy's law and the volume fractions of three levels of pores (macro-, meso- and micropores) is proposed. Then, the following results are obtained: The fundamental solution of the governing system of steady vibration equations in the considered theory is constructed explicitly by using elementary functions. Green' s formulae are obtained and the uniqueness theorems for classical solutions of the BVPs are proved. The basic properties of surface and volume potentials in the 3D linear coupled theory of thermoelasticity for materials with triple porosity are established. The existence theorems for classical solutions of the BVPs of steady vibrations in this theory are proved by using the potential method and the theory of the singular integral equations.

Acknowledgments This work was supported by Shota Rustaveli National Science Foundation of Georgia (SRNSFG) [Project # STEM-22-557].

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CT 03

	Monday
Room	CR 10 B
17:20-17:45	Joao V. Fontana
17:45-18:10	Johanna Heidrich
18:10-18:35	Fadi Awawdeh
18:35-19:00	Eleni Theodosiou

ARBITRARILY HIGH ORDER SCHEMES FOR FRACTIONAL DIFFERENTIAL EQUATIONS

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The application of fractional differential equations (FDEs) to model a broad range of phenomena has become more commonplace over the past few decades. These models are being used to examine phenomena such as anomalous diffusion in viscoelastic materials, the spread and motion of pollutants in porous media, groundwater flow, soil moisture dynamics, fractional quantum mechanics, and dynamic systems with memory or non-local properties, etc [1]. In this work, we propose high-order computational schemes for solving nonlinear FDEs. From the known structure of the smooth solution, we show that the solutions of such FDEs are equivalent to those of Volterra integral equations (VIEs). The fractional integral appearing in the integral form of the resulting VIE is then split into a history term and a local term. Subsequently, we develop an efficient strategy that utilizes a combination of a kernel compression scheme and an integral deferred correction (IDC) scheme to obtain a high-order solution. The kernel compression scheme [2] reduces the costs in approximating the history term, while the IDC scheme [3] approximates VIEs on short intervals to obtain the local information. Error analysis shows high-order accuracy of the proposed schemes. Numerical applications illustrate the effectiveness of the proposed schemes, especially for nonlinear FDEs. The results suggest that the proposed scheme provides accurate solutions even for large time steps, making it a valuable tool for researchers and engineers working on systems with memory or long-term behavior [4].

Acknowledgments The author is grateful for the support of the Scientific fund from the Hashemite University (grant 12/2021).

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CONTROL-BASED METHODS FOR MODEL VALIDATION IN FLUID DYNAMICS

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Most models of physical systems are validated by comparing stable steady states with experimental results. Unstable steady states are typically not used for validation, since they are difficult to observe experimentally. The methods of feedback control and control-based continuation (CBC) [1] can be utilized to find and stabilize unstable steady states of experimental non-linear physical systems. In feedback control, actuation is exerted onto the system, based on a measure of the difference between the system state and a prescribed target state. In CBC, which relies on feedback control, the steady solutions are calculated as function of the prescribed target state. In this study, we investigate how control-based methods can be utilized to reveal unstable steady states of the propagation of bubbles within a Hele-Shaw channel. This system is an appealing prototype for CBC: (i) it presents strong non-linear behaviour, (ii) it is a continuous system, while most systems on which CBC is utilized have few degrees of freedom, and (iii) there is a depth-averaged model [2] that presents multiplicity of solutions, both stable and unstable. Additionally, our depth-averaged model of the system is validated experimentally. We use finite element (FE) numerical simulations to design and test a suitable feedback actuation that could be used in an experimental realization of this system. Such realization would permit the direct experimental observation of unstable steady states, and the validation of the unstable solutions of our depth-averaged model.

Acknowledgments The authors are grateful for the support of Engineeering and Physical Sciences Research Council (EPSRC). (grant EP/T021365/1).

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STOCHASTIC OPTIMAL CONTROL OF DISTRICT HEATING NETWORKS UNDER DEMAND UNCERTAINTY

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Operators of district heating networks are facing numerous technical challenges in course of the energy system transformation, which require innovations in network control. A realistic mapping of the energy transport through the distribution network is key to optimizing the use of operating resources. The underlying thermo-hydraulic PDE system strongly depends on the demand resulting from the heat consumers' behavior as a boundary condition [1], and consequently the demand has a considerable impact on optimization problems constrained by this PDE system as well. As most district heating networks are equipped with little sensor technology, real-time monitoring data from heat consumers is rarely available to calibrate the simulation, and regardless of the data situation, for predictive optimization a demand forecasting needs to be provided. For these reasons, a realistic time-resolved demand prognosis has to be derived from the limited historical data available. First, underlying patterns need to be identified. Using regression analysis of historical real monitoring data of different building types over the course of different seasons, we generate temperature-dependent, time-resolved, characteristic demand profiles of heat consumers. Next, we aim to incorporate the inherent stochastic nature of demand into our previous results. As underlying patterns can be recognized and demand only takes values in a bounded interval, we find the Jacobi process to be a stochastic process that captures these characteristics. We focus on Jacobi processes with time-dependent mean reversion levels, namely the demand profiles obtained above, and provide parameter fittings for different building types. By applying the strategy presented here, a realistic time-resolved demand can be simulated only based on characteristic consumer variables.

Taking the consumers' inherently random behavior as solutions to stochastic differential equations into account, we intend to investigate its impact on the optimization results. The optimal control problem under consideration is to find the optimal input into the system such that not only the variables considered before are minimized but in addition the stochastic demands are satisfied. Propagating the uncertainty in its boundary condition through the PDE then results in a random field PDE solution and thus the objective function becomes a random variable, on which different risk measures could be applied for risk-neutral or risk-averse optimization. Solving such stochastic optimal control problems is not trivial, therefore we employ different strategies, e.g. a space mapping approach, and compare them regarding performance, computing time and robustness for our application example of a district heating network.

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AN EFFICIENT TWO DERIVATIVE IMEX SCHEME

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For time-dependent differential equations, multi-derivative methods can be an efficient option for time integration. In this context, the term multi-derivative refers to the usage of higher-order temporal derivatives of the unknown of the solution. For example, for the ordinary differential equation $\dot{w}(t) = Q(w(t))$, a multi-derivative method not only uses $Q(w)$, but also the term $Q'(w)Q(w)$, being $\ddot{w}$, and possibly higher-order versions thereof.

Using this approach, one can derive higher-order methods with fewer stages than, for example, the classical Runge-Kutta schemes. Therefore the most important advantages of the multi-derivative methods are storage efficiency while maintaining high-order accuracy.

In particular for very stiff ordinary or partial differential equations, one often resorts to implicit or implicit-explicit (IMEX) methods. In the case of an IMEX splitting, the usual procedure is to split the right-hand side into two contributions, namely one containing stiff and one contains the non-stiff parts. Very often, the nonlinearities are hidden in the non-stiff part.

However, there is a downside in the IMEX case using multi-derivative methods. It has been noticed that because of the calculation of the higher-order temporal derivative of the explicit part, the explicit part has to be inverted in the algorithm [1]. That means that the advantages that come from the explicitness, such as temporal and computational efficiency, are lost.

This presentation will focus on an efficient two-derivative IMEX scheme. This new IMEX scheme aims to exploit all the advantages of an explicit part in a multi-derivative method by modifying the standard procedure of computing the second derivative. The asymptotic preserving property of the method is explored in the solution of singularly perturbed equations, and numerical results are presented using high-order two-derivative methods to compute various differential equations. The presentation follows the results of [1].

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CT 04

	Monday
Room	CR 10 D
17:20-17:45	Shuenn-Yih Chang
17:45-18:10	Imre Fekete
18:10-18:35	Stephan Scholz
18:35-19:00	Maximilian Reiter

PROBLEM-DEPENDENT METHODS FOR SOLVING ORDINARY DIFFERENTIAL EQUATIONS

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A novel type of problem-dependent methods is derived from an eigen-based theory. Unlike the adoption of scalar constant coefficients for developing conventional solution methods, it may adopt problem-dependent coefficients. These coefficients are functions of the physical properties of the problem under analysis and therefore they have a matrix form for systems of ordinary differential equations. There are three major steps of the methodology for developing problem-dependent methods. [1] The problem that is a coupled system of ODEs is decomposed into a set of uncoupled ODEs; (2) An eigen-dependent method is developed to solve each uncoupled ODE; and (3) It is required to convert all the eigen-dependent methods to a problem-dependent method by using a reverse eigen-decomposition technique. The third step plays the key issue to facilitate the problem-dependent methods for practical applications. This is because the methodology looks like a modal analysis and it involves eigendata for decomposition and superposition. Hence, it is required to solve an eigenvalue problem to yield the eigendata for each step. Since it is very time consuming for solving an eigenvalue problem, the conversion of the third step is intended to avoid the use of eigendata. This methodology is not only for developing first order solvers [1,2] but also second order solvers [3] without reducing second order ODEs to first order ODEs. Two problem-dependent methods will be presented. One is for solving systems of ODEs of first order and the other is for solving systems of ODEs of second order. Both methods are characterized by problem dependent but not eigen dependent because that their coefficients are functions of the physical properties of the problem under analysis. Both problem-dependent methods can have an A-stability, an explicit implementation and a second order accuracy. An A-stability implies that the two methods have no limitaion on step size based on stability consideration. An explicit implementation implies that they can have a non-iterative solution procedure. A second order accuracy allow them to yield an accurate solution by using a reasonable step size. As a consequence, they are very promising for solving stiff systems of nonlinear ODEs. Numerical properties of the two problem-dependent methods will be analytically derived and numerical examples will be used to affirm these properties.

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LINEAR MULTISTEP METHODS AND RICHARDSON EXTRAPOLATION

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In this talk, we study the application the classical Richardson extrapolation (RE) technique to accelerate the convergence of sequences resulting from linear multistep methods (LMMs) for solving initial-value problems of systems of ordinary differential equations numerically. The advantage of the LMM-RE approach is that the combined method possesses higher order and favorable linear stability properties in terms of A- or $A(\alpha)$-stability, and existing LMM codes can be used without any modification.

This is a joint work with Lajos Lóczi (ELTE Eötvös Loránd University, Hungary and BME Budapest University of Technology and Economics, Hungary). The main results are based on the paper [1] and on the ongoing research project.

Acknowledgments The author was supported by the ÚNKP-22-5 New National Excellence Program of the Ministry for Culture and Innovation from the source of the National Research, Development and Innovation Fund.

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FAST COMPUTATION OF FUNCTION COMPOSITION DERIVATIVES FOR FLATNESS-BASED CONTROL OF DIFFUSION PROBLEMS

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The chain rule is a standard tool in differential calculus to find derivatives of composite functions. Faà di Bruno's formula is a generalization of the chain rule and states a method to find high-order derivatives. In this contribution, we propose an algorithm based on Faà di Bruno's formula and Bell polynomials [1,2] to compute the structure of derivatives of function compositions. The application of our method is showcased using trajectory planning for the heat equation [3].

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NUMERICAL APPROXIMATION OF GENERALIZED SOLUTIONS TO THE ERICKSEN–LESLIE EQUATIONS

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The fluid flow of the nematic phase of liquid crystals can be described by the Ericksen–Leslie system. We define the concept of energy-variational solutions for the Ericksen–Leslie equations in three spatial dimensions. This solution concept is finer than dissipative solutions and satisfies the weak-strong uniqueness property. For a certain choice of the regularity weight, we construct an energy-variational solution with the help of an implementable, structure-inheriting space-time discretization. The proposed scheme implements the main properties of the continuous system including the unit-norm restriction at every node of the mesh. Computational studies are performed in order to provide some evidence of the applicability of the proposed algorithm. A publication is available [1].

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CT 05

	Tuesday
Room	CR 114
15:30-15:55	Viktor Skorniakov
15:55-16:20	Pietari Mönkkönen
16:20-16:45	Pratik Mullick

MONTE CARLO FOLIAGE GENERATION ON 3D TREE MODELS

Pietari Mönkkönen, **Simo Ali-Löytty** and **Pasi Raumonen**

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Foliage is an important way for trees to interact with their environment, and the amount and distribution of leaf material in a tree is linked to, e.g., light transmission. The high variability in the structure among trees and the large number of individual leaves in a single tree pose a challenge on measuring the leaves. Traditionally leaf measurement have been done manually, which is labor intensive and destructive. Remote sensing of trees has proved to be useful in leaf measurements and been used to measure distribution of leaf area [1]. A notable deficiency in remote sensing methods determining leaf distributions is the lack of validation data. Simulating the remote sensing measurements to produce validation data presents an alternative approach, but it requires methods for generating tree models with foliage accurately following user defined distributions. Foliage of a tree is characterized stochastically by three distributions: leaf area density, leaf orientation and leaf size distributions. Leaf area density distribution dictates the positioning of leaves on the tree, whereas leaf orientation and size distributions define the directions of leaf normals and the sizes of individual leaves, respectively.

We present an algorithm, building on a previous method [2], for generating foliage as explicit surface models corresponding to individual leaves on a 3D tree model. It uses Monte Carlo sampling of the individual leaves from user defined foliage distributions. The 3D branching structure of the tree is represented with quantitative structure models (QSMs), which are hierachical collection of cylinders [2]. The leaf area density depends on three variables of tree structure: vertical position, position on branch, and the azimuthal direction seen from the stem. The marginal distribution options for these variables include, e.g., beta, Weibull, and Von Mises distributions. The leaf orientation distribution depends on the vertical position and can be set to follow, e.g., de Wit's distributions [3] which can change their shape vertically along the tree model.

Our approach combining 3D tree model and continuous leaf distributions for area density, orientation and size provides a generalizable and tree structure dependent framework of leaf distribution representation. The tree-leaf model produced by our algorithm can be used in remote sensing simulations and the resulting data can be exploited for multiple purposes, e.g., validating the accuracy of the remote sensing methods or developing more accurate inversion methods to infer leaf distributions.

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COMPUTATIONAL STRATEGIES FOR ANALYZING COLLECTIVE BEHAVIOR IN HUMAN CROWDS

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The collective motion of social agents that arises from their interactions has been the subject of intense scientific research. Understanding the collective dynamics of human crowds is critical for improving pedestrian traffic flow, ensuring crowd safety, effective urban planning, and preventing crowd disasters. In particular, the analysis of real-life mass events, such as religious gatherings, music concerts, sporting matches, and transportation hubs, has been essential for modeling crowd behavior with the goal of preventing life-threatening situations such as crushes, stampedes, and trampling. Analyzing crowd dynamics and pattern formation in human data is a crucial first step towards a successful human-crowd modeling.

To understand the crowd behavior one has to rely on experimental data using real human beings. Pedestrian traffic flow has been studied empirically in a wide variety of situations, using both experimental methods and motion tracking of real crowds. When two streams of pedestrians cross at an angle, striped patterns spontaneously emerge as a result of local pedestrian interactions. Several urban situations produce crossing flows, such as streams of pedestrians crossing at a sidewalk intersection, or subway commuters passing each other when entering and exiting a public transport, such as a metro car. It is very common to notice that pedestrians in a crosswalk often form multiple lanes of traffic. Such spontaneous pattern formation is an example of self-organized collective behavior, a topic of intense interdisciplinary interest.

In this contributed talk, I wish to present numerical strategies that were developed to study the geometric properties of striped patterns, which arise as a consequence of two crossing flows. In [1], we presented two novel computational methods for analyzing striped patterns in pedestrian data: (i) an edge-cutting algorithm, which detects the dynamic formation of stripes and allows us to measure local properties of individual stripes; and (ii) a pattern-matching technique, based on the Gabor function, which allows us to estimate global properties of the striped pattern at a time. We found an invariant property: stripes in the two groups are parallel and perpendicular to the bisector at all crossing angles. I shall also present our ongoing research, where we are working on another elegant approach to detect the stripes using matrices constructed out of the crossing information of two agents from opposite groups.

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ON THE OPTIMAL PAIRWISE GROUP TESTING ALGORITHM

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An idea of Group Testing (GT) was first announced by Dorfman [1] in 1943 as a cost saving way for biomedical screening. It was later expanded by many others and brought to very different fields. In our talk, we cover the GT idea, discuss main questions and problems related to application of a typical GT algorithm, and end up with a highlight of our recent results [2] on the Pairwise Testing Algorithm proposed by Yao and Hwang [3].

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CT 06

	Wednesday
Room	CR 113
15:30-15:55	Willem Jansen
15:55-16:20	Sanjana Verma
16:20-16:45	Sandeep Kumar

CONCATENATED BACKWARD RAY MAPPING ON THE COMPOUND PARABOLIC CONCENTRATOR

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Concatenated backward ray mapping [1] is an alternative for ray tracing to compute the light distribution at the target of an optical system given a source distribution. A common 2D ray tracing algorithm used in industry is Monte Carlo (MC) ray tracing which is slow and not very accurate. Concatenated backward ray mapping uses the phase spaces of *all* surfaces of the optical system to compute the light distribution; which is shown to be faster and more accurate.

Phase space (PS) [2] is the set of position and direction coordinates of rays intersecting a surface. In 2D a surface reduces to a line, the position is the x-coordinate of the intersection and the direction is the sine of the angle between the ray and the surface normal. Phase spaces are partially empty; non-empty regions account for light emitted by the source. The phase spaces of the optical system are connected through maps that relate the coordinates on every PS.

Concatenated backward ray mapping requires much fewer rays to compute the light distribution. This is achieved by only tracing light on the boundaries of the non-empty regions in PS from the target back to the source using the inverses of the maps. When light from the boundaries reaches the source it is traced to the target.

We extend concatenated backward ray mapping to accommodate curved segments as the original algorithm is limited to only straight line segments. The extended backward algorithm is applied to the compound parabolic concentrator (CPC) [3], a standard 2D optical system which collects parallel light and reshapes it to a focused beam.

We compare the accuracy and speed of the extended algorithm to the previously introduced algorithm [1] and MC ray tracing. We compare them on the CPC and on a discretized CPC. The accuracy of the algorithms is determined by the difference between the results and a reference solution.

Preliminary tests show that the extended algorithm outperforms MC ray tracing on the CPC, both in accuracy and speed. On the discrete CPC the extended algorithm performs similar to the previously introduced algorithm.

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LAGRANGIAN COHERENT STRUCTURES IN LAPAROSCOPIC SURGERY

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Laparoscopy is an electrosurgical medical operation involving an application of high-frequency alternating current to remove the undesired biological tissue from the insufflated abdomen accessible through inlet and outlet trocars. One of the main byproducts in this process is the gaseous particles, called surgical smoke which is found hazardous for both the patient and the operating room staff. The elimination of this hazardous material is an area of active research in the medical community. Thus, understanding their dynamics influenced by the underlying flow inside the abdomen is crucial.

In this talk, we present a computational fluid dynamics model and analyse the velocity field through the Lagrangian Coherent Structures (LCS) technique in an insufflated abdomen-shaped geometry. We show that in this way, regions with different vortex boundaries are detected which are responsible for the transportation and mixing of the material particles in the flow. These boundaries are dependent on the angle, positions, and number of the outlets and inlets and thus, provide a novel utility of LCS in medical surgery that can detail the dynamics of surgical smoke and are capable of informing a better design of effective smoke removal technologies.

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TWO-DIMENSIONAL FREEFORM REFLECTOR DESIGN FOR MINIMIZING ABERRATIONS

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The objective of this talk is to use the techniques from illumination optics to optimize imaging systems. In illumination optics, freeform surfaces are computed for specified source and desired target light distributions [1]. For two-dimensional systems, the shape of a reflector is the solution of an ordinary differential equation, which is determined by combining the optical map and conservation of energy. In imaging optical systems, aberrations are deviations from ideal imaging and they degrade the quality of an image. Freeform surfaces are commonly used for minimizing aberrations. They are the most preferred choice because they provide a higher degree of flexibility in optical design compared to simple conic shapes, due to lack of symmetry.

When off-axis rays pass through an optical system, they form an aberrated spot in the image plane. The size of the spot, called the root-mean-square (RMS) spot size, quantifies aberrations. We focus on designing an optical system consisting of freeform reflectors that can minimize aberrations for multiple sets of off-axis parallel light beams. The RMS spot size is estimated by the standard deviation of the target coordinates obtained by ray tracing. We subsequently take the RMS of the spot sizes generated by various parallel ray collections. This determines the deviation in aberrations of on-axis and off-axis light beams. It is a merit function that depends on the energy distributions at the source and target of the optical system. This is because all ray beams pass through an optical system computed using certain energy distributions at the source and target. We minimize the merit function using the derivative-free Nelder-Mead optimization algorithm [2]. The minimization facilitates in finding the optimal energy distributions. They in turn enable us to determine the freeform reflectors which ensure the least changes in spot sizes among all sets of parallel off-axis rays.

We test our approach for two configurations, first, a parallel source to a near-field target consisting of a single reflector, and second, a parallel source to a point target consisting of two reflectors. The two-reflector system is better than the single-reflector system in minimizing the aberrations of off-axis rays.

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CT 07

	Tuesday
Room	CR 114
17:20-17:45	Juancho Collera
17:45-18:10	Lukas Kannengießer
18:10-18:35	Barbara Zubik-Kowal
18:35-19:00	M. Filomena Teodoro

COUPLED DELAYED ACTION OSCILLATOR MODEL OF THE ENSO

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Drastic fluctuations in sea-surface temperature (SST) may cause massive rainfall which causes severe floods, as well as extreme drought which increases the occurrence of forest fires. In [1], Suarez and Schopf introduced the delayed-action oscillator (DAO) model to describe the irregular fluctuations of the SST on a region in the central equatorial Pacific that has a strong ocean-atmosphere coupling. Their model incorporates the effects of oceanic wave transit and helps to explain the El Niño-Southern Oscillation (ENSO) phenomenon. In a more recent work, Boutle et al. [2] studied the influence of the annual cycle, global warming, and stochasticity in the DAO model. In the same study, a model of a coupled DAO was introduced which describes the scenario where there are two coupled regions along the equatorial Pacific with strong ocean-atmosphere coupling. Numerical simulations show that the behavior obtained from the coupled DAO is more similar to that of the El Niño than the behavior from the simple DAO. In this talk, we revisit the coupled DAO model and explain why it is better at describing the fluctuations in SST during El Niño events. Particularly, we examine the different periodic solutions of the coupled DAO model which can emerge from the limit-cycle bifurcations.

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PARAMETER IDENTIFICATION IN BOUNDARY VALUE PROBLEMS FOR FIBER SPINNING

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Material behavior in industrial manufacturing processes can often be described by a system of differential equations with respective material laws. Since these material laws depend on material-specific parameters, which are frequently unknown or can only be obtained through a range of expensive experiments, there is a need for numerical parameter estimation strategies. In this context, we consider a process described by a boundary value problem (BVP) of ordinary differential equations where some model parameters need to be estimated on the basis of few experimental data. Computing numerical solutions is very demanding, and disconnecting the parameter estimation from the solution approach of the BVP leads to a time-inefficient estimation strategy. Therefore, we propose a method that, given a set of experimental measurements, efficiently estimates the specific material parameters by connecting the used continuation method for solving the BVP with a trust region method. Furthermore, we demonstrate the method's success in a parameter identification problem arising in industrial fiber spinning processes.

BAROTRAUMA, A POSSIBLE MODEL

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The purpose of this work was to determine the incidence and severity of the barotrauma and to identify the possibility of middle ear barotrauma in a high number of patients undergoing regular hyperbaric oxygen therapy. To explore and clarify this issue in terms of incident, were registered seriousness and recurrence, age, gender, clinical signs, specific history of chronic rhinitis and symptoms of nasal obstruction during the occurrence. A first approach was performed by the authors where a descriptive statistical analysis and some elementary and intermediate statistical techniques such an variance analysis were performed. In the actual work and as continuation of [1], [2] a Logit model was explored allowing to relate the occurrence of barotrauma with the clinical profile of patients. We could conclude that Hyperbaric Oxygen Therapy is safe.

Acknowledgments This work was supported by Portuguese funds through the Center for Compu-tational and Stochastic Mathematics (CEMAT), The Portuguese Foundation for Science and Technology (FCT), University of Lisbon, Portugal, project UID/Multi/04621/2019, and Center of Naval Research (CINAV), Naval Academy, Portuguese Navy, Portugal.

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ITERATIVE SOLUTION TECHNIQUES BASED ON THE MAGNITUDES OF PHYSICAL PARAMETERS APPEARING IN GIVEN DIFFERENTIAL SYSTEMS

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Numerous mathematical models applied to solve real-world problems are written in terms of systems of differential equations involving physical parameters of magnitudes oscillating between small and large numbers. Such differences in the orders of magnitude often make it difficult to solve many differential systems. In this work, we present mathematical techniques that allow to employ such differences in the magnitudes of the given parameters in order to accelerate the convergence of dynamic iterations applied to differential systems formulated in terms of these parameters.

Dynamic iterations differ from static iterations in that they involve time-dependent vectors, allowing to simplify the original differential systems. These simplifications bring diverse advantages. For example, the application of dynamic iterations allows to transform systems of nonlinear differential equations into systems of linear differential equations. Another advantage is that dynamic iterations allow to apply implicit time integration methods without having to solve algebraic systems at each time step. Dynamic iterations allow also to divide a given system into simpler subsystems that can be solved in parallel computing environments.

In this work, we analyze the relationship between the errors of successive dynamic iterates and the magnitudes of the model parameters in order to speed up the convergence of the iterations. We combine the designed iterative scheme with implicit methods and propose a numerical algorithm to solve linear and nonlinear systems of differential equations. Numerical experiments are presented to demonstrate the efficiency of the algorithm.

CT 08

	Wednesday
Room	CR 113
10:40-11:05	Hasifa Nampala
11:05-11:30	Giuseppe Pontrelli
11:30-11:55	Giulia Elena Aliffi
11:55-12:20	Kevin Moroney

A SYSTEM OF RANDOM ODES FOR REPRESENTING TRENDS OF CGM SIGNALS

Giulia Elena Aliffi[a], **Giovanni Nastasi**[a], **Vittorio Romano**[a], **Dario Pitocco**[b], **Alessandro Rizzi**[b], **Elvin J. Moore**[c], **Andrea De Gaetano**[d,e,f]

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Diabetes Mellitus is a metabolic disorder which may result in severe and potentially fatal complications if not well-treated and monitored. In this study, a quantitative analysis of the data collected using CGM (Continuous Glucose Monitoring) devices from six subjects with type 2 diabetes in good metabolic control at the University Polyclinic Agostino Gemelli, Catholic University of the Sacred Heart, was carried out. In particular, we expanded on the deterministic first-order differential equation model proposed in [1] and we proposed a system of random ordinary differential equations whose state variables are affected by a sequence of stochastic perturbations to extract more informative inferences from the patients' data [2]. For this work, Matlab and R programs were used to find the most appropriate values of parameters (according to the Akaike Information Criterion (AIC) and the Bayesian Information Criterion (BIC)) in models for each patient. Specifically, the fitting was carried out by using the Particle Swarm Optimization Method to minimize the ordinary least squares error between the observed CGM data and the data from the random ODE model. Goodness of fit tests were made in order to assess whether or not the exponential distribution, whose parameter had been estimated by Maximum Likelihood Estimation, was suitable for representing the waiting times computed from the model parameters. Finally, both parametric and non-parametric density estimation of the frequency histograms associated with the variability of the glucose elimination rate from blood into the external environment were conducted and their representative parameters assessed from the data. The results show that the chosen models succeed in capturing most of the glucose fluctuations for almost every patient.

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MATHEMATICAL MODELLING OF DRUG RELEASE FROM PHARMACEUTICAL GRANULES IN DISSOLUTION TESTING

Kevin Moroney[a,b], **Milton Assunção**[a,b] and **Michael Vynnycky**[a,b]

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Standardised *in vitro* dissolution testing is used to understand and design pharmaceutical oral solid dosage forms, such as tablets and capsules, in a laboratory setting. By systematically testing various product formulations consisting of active drug and different filler (excipient) materials within the allowable design space, the physical and chemical properties are altered to achieve a targeted drug release profile over time. Nevertheless, the observed release profile may arise from a combination of several physicochemical processes, so it is difficult to gain a comprehensive understanding of the release behaviour without extensive testing and trial and error. Thus, the ability to mathematically model these processes accurately is important to understand how the formulation parameters can be adjusted to control the release. In this work, we consider drug release from a porous drug-excipient granule or population of granules. A model explicitly accounting for drug solubility limitations and certain microstructural variations within the granule(s), factors that are commonly neglected in other models, was presented recently [1,2]. Here we consider some different applications of this model to situations which arise in dissolution testing. The model is analysed in different regimes of interest including cases where so-called 'sink' conditions are not valid [3]. The general model requires the solution of a moving boundary value problem but it is sufficient to solve a reduced model in some case of practical interest. Some comparisons of the model to experimental data from [4] will be presented and model extensions will be discussed.

Acknowledgments The authors are grateful for the research support provided in part by a grant from Science Foundation Ireland co-funded under the European Regional Development Fund under Grant number 12/RC/2275_P2.

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ANALYSIS OF HIV THERAPY IN THE LIVER USING OPTIMAL CONTROL AND PHARMACOKINETICS

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The main burden in treating human immunodeficiency virus (HIV) infection currently, is the side effects of the antiretroviral therapy (ART) used, because each treatment is toxic to the liver [1]. This study uses optimal control theory applied to a mathematical model that describes the dynamics of HIV infection in the liver. The optimal controls are presented as therapy efficacy of reverse transcriptase inhibitors (RTIs), integrase inhibitors (INs) and protease inhibitors (PIs) [2]. An objective function is defined with an aim to investigate the optimal control strategy that minimises toxicity [3], viral load and cost of first-line and second-line HIV regimen. Our results indicate, that in the first-line regimen with INs, a patient has to take medication for at least 98% of the treatment time and the regimen should be close to 100% efficacious regardless of the intervention cost. For second-line regimen, the period of drug administration of PIs largely depends on the weight constants. Inclusion of INs in the first-line regimen yields better HIV DNA suppression, as they are more efficacious than NRTIs. Defining toxicity and efficacy using pharmacokinetic parameters of all drugs studied [4], nevirapine is highly efficacious and most toxic. The study recommends routine transaminase tests because results indicate liver enzyme elevation even with very low viral load.

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MODELLING SMART DRUG RELEASE WITH FUNCTIONALLY GRADED MATERIALS

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Technological advances over the past decades have led to the development of sophisticated drug delivery devices that enable targeting and control of drug delivery [1]. A better controlled and personalized release is often desired and many new technologies and strategies are being developed to try to address this objective.

Recently, more attention has been paid to functionally graded materials (FGMs), a variety of composite materials in which the constitutive properties vary smoothly and continuously from one region to another [2].

Through a mathematical mechanistic model and a simulation approach, we explore the potential of FGMs as a new class of controlled drug delivery materials, in the attempt to establish whether varying shape material properties can provide an advantage over homogeneous medium. We develop a continuum model to describe drug transport within, and release from, a FGM drug-eluting stent system. A numerical solution is presented and the differences and the potential of functionalized release over a homogenous stent coating are outlined.

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CT 09

	Wednesday
Room	CR 106
10:40-11:05	Omar Alsayyed
11:05-11:30	Juan Rocha
11:30-11:55	Daniel Booth
11:55-12:20	Anna Szafrańska

REGULARIZATION METHODS FOR SOLVING INVERSE PROBLEMS

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Inverse problems are a class of mathematical problems that aim to recover the unknown causes or parameters of a system from observable data. These problems arise in various fields, including engineering, physics, geophysics, medical imaging, and more [1]. Inverse problems are ill-posed problems, meaning they are often challenging to solve due to their unstable nature. Regularization methods are widely used to address the instability of inverse problems [2]. These methods aim to reduce the noise or error in the data while still preserving the important features of the solution. In this talk, we will discuss some of the most common regularization methods used for solving inverse problems. The most popular regularization method for solving inverse problems is Tikhonov regularization. This method adds a regularization term to the objective function, which penalizes the solution for being too complex. The regularization term acts as a constraint on the solution, ensuring that it is smooth and avoids sharp changes. The strength of the regularization is controlled by a regularization parameter, which determines the trade-off between fitting the data and minimizing the regularization term. Another common regularization method is total variation (TV) regularization. TV regularization seeks to preserve the edges and sharp features in the solution while still reducing noise. The method penalizes the variation or gradient of the solution, promoting solutions with sharp transitions. TV regularization has been applied to many image processing and computer vision applications and has been shown to produce visually pleasing results. More advanced regularization methods include wavelet regularization and sparsity-promoting regularization. Wavelet regularization uses wavelet transforms to decompose the solution into different frequency bands and applies different regularization strengths to each band. This method is particularly useful for image processing applications where the solution contains both smooth and oscillatory components. Sparsity-promoting regularization methods promote solutions that are sparse or have only a few non-zero coefficients. This approach has been particularly useful in signal processing applications, where the signals are sparse in some domain. The choice of regularization method depends on the specific application and the properties of the solution we want to obtain [3].

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A HELE-SHAW NEWTON'S CRADLE: CIRCULAR BUBBLES IN A HELE-SHAW CHANNEL

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We present a model for the motion of approximately circular bubbles in a Hele-Shaw cell. The bubble velocity is determined by a balance between the hydrodynamic pressures from the external flow and the drag due to the thin films above and below the bubble. We find that the qualitative behaviour depends on a dimensionless parameter $\delta \propto \mathrm{Ca}^{1/3} R/h$, where Ca is the capillary number, R is the bubble radius and h is the cell height. An isolated bubble travels faster than the external fluid if $\delta > 1$ or slower if $\delta < 1$, and the theoretical dependence of the bubble velocity on δ is found to agree well with experimental observations. Furthermore, we show how the effects of interaction with cell boundaries and/or other bubbles also depend on the value of δ. For example, in a train of three identical bubbles travelling along the centre line, the middle bubble either catches up with the one in front (if $\delta > 1$) or is caught by the one behind (if $\delta < 1$), forming what we term a Hele-Shaw Newton's cradle.

MAXIMUM PRINCIPLE FOR TIME-FRACTIONAL DIFFUSION EQUATIONS WITH THE CAPUTO-KATUGAMPOLA DERIVATIVE

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In this contributed talk, we present maximum principle for a time-fractional Caputo-Katugampola diffusion equation. In addition, we prove some results on the uniqueness of the solutions and about the continuity of the solutions with respect to the boundary conditions.

Acknowledgments The first, second and fifth authors are partially supported by the project $PID2019 - 106093GB - 100$.

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FRACTIONAL MODELING WITH APPLICATION IN BIOLOGY

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Modeling of natural phenomena like e.g. spread of the virus or interactions between species, using mathematical tools is highly desirable due to the possibility of understanding and analyzing the problem. A well-constructed model can be used to observe and predict the dynamics of a given phenomenon. The usual tools based on ordinary or partial differential equations in some cases can be insufficient to capture well the dynamic behavior, especially in the modeling phenomena where we are dealing with the memory effect. To deal with this problem we can successfully reach for the fractional calculus and take advantage of the non-locality property of the fractional order derivatives. Moreover, not without significance is choosing appropriate numerical scheme for solving fractional differential problems.

In this talk we give some examples of superiority of mathematical modeling using fractional calculus over the classical approach. We also present an appropriate construction of the numerical scheme, in order to preserve the most important properties of the modeled phenomenon [1].

In particular, we provide an example of an approach to modeling the course of an epidemic caused by the dengue virus, i.e. fractional model construction, numerical approach for model validation, parameters identification [2].

Acknowledgments A. Szafrańska thanks the National Science Center for the financial support, under the research project No. 2021/05/X/ST1/00332.

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CT 11

	Wednesday
Room	CR 106
15:30-15:55	Joe Roberts
15:55-16:20	Shahid Mubasshar
16:20-16:45	Roberto Beneduci
16:45-17:10	Milton Assunção

FOREST FIRES SPREADING: A NON-LINEAR PROBABILISTIC CONTINUOUS SPACE-TIME MODEL

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Forest fires management is an ever more important factor in the human effort to preserve biota and to mitigate climate change. Stochastic models are particularly appropriate to describe forest fire spreading since the latter is a complex phenomena characterized by a stochastic behavior. Nowadays, the enormous quantity of georeferenced data and the availability of powerful technics for their analysis can provide a very careful picture of forest fires. We propose a stochastic spreading model continuous in space and time that is able to use such data in their full power. It is a kind of mother model from which many other models (both stochastic and deterministic) can be derived providing a unified approach. For example, stochastic models based on cellular automata can be derived by time and/or space discretization. The model is inspired by the epidemic model developed in [1]. In order to outline its main features, let us consider a surface Σ on the earth, a point in Σ being denoted by $\boldsymbol{x} = (x, y) \in \Sigma$. We assume there are positive definite functions $\psi^F(t, \boldsymbol{x}), \psi^B(t, \boldsymbol{x}), \psi^G(t, \boldsymbol{x}) \in L^1(\Sigma, d^2\boldsymbol{x})$ representing sub-probability densities and describing the state of the forest fire at time t. In particular, $\psi^F(t, \boldsymbol{x})$ is the sub-probability density for the trees on fire, $\psi^B(t, \boldsymbol{x})$ the sub-probability density for the burnt trees (firing trees which turned into burnt trees) and $\psi^G(t, \boldsymbol{x})$ the sub-probability density of the green trees. Their sum satisfies $\int_\Sigma [\psi^F(t, \boldsymbol{x}) + \psi^B(t, \boldsymbol{x}) + \psi^G(t, \boldsymbol{x})] d^2\boldsymbol{x} = 1$. The time evolution of the state is given by a non-linear system of integro-differential equations for $\psi^F(t, \boldsymbol{x}), \psi^B(t, \boldsymbol{x}), \psi^G(t, \boldsymbol{x})$

$$\frac{\partial \psi^F(t, \boldsymbol{x})}{\partial t} = -\alpha(t, \boldsymbol{x})\psi^F(t, \boldsymbol{x}) + \psi^G(t, \boldsymbol{x}) \int_\Sigma W(t, \boldsymbol{x}, \boldsymbol{x}_1)\psi^G(t, \boldsymbol{x}_1) d^2\boldsymbol{x}_1$$

$$\frac{\partial \psi^G(t, \boldsymbol{x})}{\partial t} = -\psi^G(t, \boldsymbol{x}) \int_\Sigma W(t, \boldsymbol{x}, \boldsymbol{x}_1) d^2\boldsymbol{x}_1$$

where α is the burning probability rate and W is the transition kernel encoding the fire spreading. Numerical implementations show forest fire behavior in several frameworks as for example the spreading through a river due to fire spotting. Real case simulation can be obtained by empirical estimation of the sub-probability density functions (by using, for example, the kernel density estimation method (KDE)) and their time evolution (provided by the model) can be used for probabilistic forecasting: to locate those regions in space where the firing probability is going to increase.

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ON THE DISSOLUTION OF PARTICLES SUBJECT TO MIXED CONVECTION

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The dissolution of a solid spherical particle is a canonical problem that is found in many industrial and consumer applications, ranging from pharmaceutical and food products, to chemicals, detergents, and paints [1]. In this scenario, the flow-through (USP) apparatus 4, is an important tool used in the pharmaceutical industry to study *in vitro* dissolution on a wide range of dosage forms including tablets, granules and powders [2]. Its assembly includes a reservoir, a pump for the dissolution medium and a flow-through cell; it operates by pumping the dissolution medium upwards through the flow-through cell, where the dosage form is allocated.

The forced convection induced by the pump, alongside the diffusion of the solute in the solvent may be regarded as the dominant mass transfer mechanisms. A recently published paper [3] established a model for the dissolution of spherical solid particles derived from fundamental conservation laws accounting the role of forced convection in the surrounding dissolving medium and causing deviations from the initial spherical geometry.

In this study, we consider an extension to that framework by incorporating the natural convection as a potentially relevant mechanism; the dissolution leads to a concentration gradient in the solvent, which drives the fluid motion. We investigate how natural and forced convection may act together to affect the hydrodynamics and how they interplay with the diffusion during dissolution to deform the particle geometry whilst altering the release profile of pharmaceutical ingredients, a key aspect in drug delivery.

Acknowledgments The authors are grateful for the research support provided in part by a grant from Science Foundation Ireland co-funded under the European Regional Development Fund under Grant number 12/RC/2275 P2.

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Carbon fibre is a very versatile material with applications in many different industries from medical, electronics, marine, to space. The demand for carbon fibre composites is increasing yearly and therefore the amount of waste carbon fibre is rising. This waste can be recovered and turned into a material that can be used in industry. The waste carbon fibre can be converted into a "nonwoven" form using a carding process. In this study, we examine the breaking up of "tows" of fibres in the carding machine by focusing on a probabilistic model. We derive a master equation for the breakup of tows in particular regions of the machine and then examine how a distribution of tows evolves as it moves through multiple of these regions. We study tow properties such as size and length, and look at how the machine properties affect the process.

NATURAL VIBRATIONS OF STEPPED NANOARCHES WITH DEFECTS

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A numerical solution is developed for clamped-simply supported nanoarches based on the non-local theory of elasticity. The research will be helpful to study the nanostructures such as micro-electromechanical systems [1]. The nanoarch under consideration has a step-wise variable cross-section and is weakened by a crack-like defect. It is assumed that the crack is stationary and the mechanical behaviour of the nanoarch can be modelled by Eringen' s non-local theory of elasticity. Materials change their physical and thermal properties when their dimension goes up to the nano level. The classical theory of elasticity is unable to describe such changes in material properties. This is because, during the development of the classical theory of elasticity, the speculation of molecular objects was avoided. Therefore, the non-local theory of elasticity is applied to study the vibration of nanostructures and it has been accepted by many researchers. In the non-local theory of elasticity, it is assumed that the stress state of the body at a given point depends on the stress state of each point of the structure. However, within the classical theory of elasticity, the stress state of the body depends only on the given point [2]. The system of main equations consists of equilibrium equations, geometrical relations and constitutive equations with boundary and intermediate conditions. The system of equations is solved by using the method of separation of variables. The influence of cracks and steps on the natural vibration of the nanoarches is prescribed with the aid of additional local compliance at the weakened cross-section. An algorithm to determine the eigenfrequencies of nanoarches is developed with the help of computer software. The effects of various physical and geometrical parameters are recorded and drawn graphically.

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CT 12

	Friday
Room	CR 113
15:30-15:55	Hoang An Tran
15:55-16:20	Bogna Jaszczak
15:55-16:20	Katarzyna Kowal

ON THE COUPLING DARCY AND FREE FLOW THROUGH A REDUCED-DIMENSIONAL BRINKMANN LAYER

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This work is motivated by the flow in ecotrons, a research facility reproducing the ecosystem at the laboratory scale, and under controlled and monitored conditions. An ecotron dome consists of three sub-domains, reproducing the atmosphere, the soil, and the canopy layer in between.

We start by presenting the mathematical model used for the numerical simulation of the moisture flow and the heat transfer in the dome. In each of the above-mentioned layers, the heat transfer is modelled by the advection-diffusion model, with layer-dependent parameters. The vapour flow in the atmosphere layer is modelled by the Navier-Stokes equations, and the Darcy law is used for the (saturated) soil. The canopy is viewed as a porous medium with a very high porosity, and the Brinkman law is used for the vapour flow. For all these layers, appropriate coupling conditions have to be considered for both moisture and heat flow.

In the Ecotron, the height of the canopy layer is much smaller than its diametre. Therefore, to increase the simulation efficiency, this layer is further reduced to a lower dimensional manifold separating the atmosphere and the soil layers. In doing so, averaging and asymptotic expansion methods are being used. The outcome is a two-layer domain (atmosphere and soil) separated by an interface. The mathematical models adopted in these two layers are coupled through the reduced dimensional model derived for the canopy layer.

The efficiency of the approach will be shown via some comparisons between non-reduced and reduced problems.

MATHEMATICAL MODELLING AND ANALYSIS OF THE FLOW OF VISCOUS FLUIDS OVER SLIPPERY SUBSTRATES

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In nature and industry, certain types of substrates promote increased fluid flow through sliding. Examples include the lotus leaf and fabricated hydrophobic surfaces, which are of use for various industrial applications, from microfluidics and flow delivery in the pharmaceutical and biotechnology industries, to drag reduction applications in the aeronautics and maritime industries, for example. What makes these types of surfaces slippery is their microstructure, which cushions the flow from below, promoting slip.

We develop a novel macroscopic mathematical model of the free-surface flow of viscous fluids over a slippery, structured substrate and investigate similarity solutions and asymptotic solutions across relevant parameter regimes. Akin to classical hydrophobic surfaces, the substrate consists of a periodic sequence of two-dimensional, fluid-filled cavities. The shear stress exerted by the overlying viscous fluid drives a return flow within each cavity. This induces a sliding velocity at the interface between the two fluids, which we determine by performing numerical simulations of the flow within each cavity. We use this sliding velocity to derive a macroscopic mathematical model of the overlying flow with basal sliding and find that the flow can be characterised in terms of a slip length proportional to the ratio of the viscosities of the two fluids. This theoretical result is confirmed by a series of fluid-mechanical laboratory experiments.

There are two asymptotic limits of our mathematical model, depending on the viscosity ratio. The first limit is a no-slip regime, valid when the viscosity of the saturating fluid is much higher than that of the overlying fluid. The second asymptotic limit is a very slippery regime, valid when the viscosity of the saturating fluid is much lower than that of the overlying fluid. Both of these regimes give rise to limiting similarity solutions. Solutions of the full mathematical model approach these two similarity solutions for low and high viscosity ratios.

Acknowledgments This work was supported by a L' Oreal-UNESCO UK and Ireland FWIS Fellowship.

MODELLING TRAIL RUNNING

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Trail running is a sport that takes place outdoors, on different types of off-road terrain such as sand, dirt roads, or forest paths, usually including significant ascents and descents. The most important question for the runner is how their pace should vary during the race to minimize the finish time. To find the optimal strategy, we have used the improved Keller's model [1]. We have added the factor representing the energy coming from carbohydrates ingestion during the race. We showed that for runs that are long enough, the effect of nutrition is the significant decrease in the time of finishing the race. Additionally, we have checked that the runner's level of endurance fitness, represented by energetic equivalent of $V\dot{O}2$, has much bigger impact on the runner's results than the initial level of anaerobic energy. We have also proposed the new model, incorporating the results of physiological experiments presented in the paper of Minetti et al. [2]. We managed to obtain much more plausible results compared to the Keller's model. We have also proposed the method to approximate the time of finishing the race given the runner's $VO\dot{2}_{\max}$ and the route specification. The percent error between the prediction and real result have not exceeded 5 % for most of the considered races.

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CT 14

	Friday
Room	CR 114
15:30-15:55	Michael Vynnycky
15:55-16:20	Luis Javier Pérez-Pérez
16:20-16:45	Maryam Ghalati

DATA-DRIVEN BOF ENDPOINT TEMPERATURE PREDICTION FOR SUSTAINABLE STEELMAKING

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Accurate endpoint temperature prediction in basic oxygen furnace (BOF) steelmaking is essential for optimizing process control, ensuring energy efficiency, and maintaining product quality, with significant implications for sustainability. In this study, we present a data-driven approach that harnesses machine learning (ML) techniques to predict the endpoint temperature in BOF steelmaking, using a large-scale, realistic dataset collected over one year from a steel company's production line. The comprehensive dataset comprises liquid iron compositions, initial temperatures, oxygen flow rates, and other relevant variables, capturing the complexity and variability inherent in steelmaking processes.

Rigorous preprocessing, ML selection techniques, and domain expertise-guided feature engineering and selection techniques were employed to identify the most influential factors for predicting endpoint temperature.

Multiple machine learning algorithms, including linear regression, support vector regressor, random forests, and neural networks, were systematically trained, tuned, and compared to determine the best-performing model for endpoint temperature prediction. The chosen model demonstrated high accuracy on unseen data, outperforming existing research. This study highlights the potential of data-driven machine-learning approaches to significantly enhance endpoint temperature prediction in BOF steelmaking using large-scale, realistic data, contributing to improved process control, energy efficiency, product quality, and overall sustainability in the steel industry.

A HIERARCHICAL MATHEMATICAL MODEL OF THE BLAST FURNACE TROUGH

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Steel manufacturing is mainly carried out using hot metal, an intermediate material produced in Blast Furnaces (BF) through the reduction of iron ore. The produced slag and hot metal in the BF are drained and collected in the Blast Furnace Trough (BFT), a refractory-lined structure that separates and transports both materials to the next stage of the process. It undergoes high rates of wear due to factors such as mechanical erosion, chemical corrosion and cyclic thermal loading due to the discontinuous BF draining process. At present, the extent to which these factors contribute to refractory wear is still not well-understood [1].

To address this issue, a hierarchy of three different mathematical models is proposed to study the thermal and hydrodynamic behaviour of the BFT. First, a CFD model is used to analyse the transient multiphase flow in the BFT during several stages of a typical BF tapping, neglecting thermal effects. The obtained velocity profile serves as the boundary condition for a second model incorporating heat transfer, aiming to assess the temperature in the solid refractories and the fluid phases assuming steady-state conditions. Finally, a simplified transient 2D thermal model is employed to investigate the effect of tapping cycle interruptions on the temperature during the BFT's two-month campaigns [2].

These mathematical models allow studying several factors related to refractory wear and tear, such as the influence of the BF tapping cycles on the wall shear stress or the cyclic thermal loading of the refractory materials.

Acknowledgments This work was partially supported by FEDER and Xunta de Galicia funds under the ED431C 2017/60 and ED431C 2021/15 grants, by the Ministerio de Ciencia, Innovación y Universidades through the Plan Nacional de I+D+i (MTM2015-68275-R) and the grant BES-2016-077228, and by the Agencia Estatal de Investigación through project PID2019-105615RB-I00/AEI / 10.13039 /501100011033.

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TOWARDS AN ASYMPTOTIC MODEL OF A BLAST FURNACE

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A blast furnace is a high-temperature bed reactor in which hot metal is rapidly and efficiently produced from ferrous materials. It is one of the most important industrial technologies for ironmaking and it is therefore natural that mathematical modelling and numerical simulation in this field has been extensive; for fairly recent comprehensive reviews, see [1,2]. In this contribution, we extend a recent asymptotic model for isothermal gas-solid flow in a countercurrent moving bed reactor [3], with a view to incorporating heat transfer [4]. Amongst other things, the model allows for conduction, convection, interphase heat transfer and thermal non-equilibrium between the two phases. In this way, we are able to provide a qualitative analysis of how the numerous model parameters, some of which are not well-known in practice, affect model predictions - in particular, the location in the furnace of the start of the cohesive zone, at which iron first begins to soften, before subsequently melting. The trends are confirmed through numerical computations of the reduced asymptotic model.

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CT 15

	Friday
Room	CR 10 D
15:30-15:55	Ann Smith
15:55-16:20	Vicky Holfeld
16:20-16:45	Simon Beckmann

INCREASING TRAINING ROBUSTNESS OF RECURRENT NEURAL NETWORKS USING PARTICLE SWARM OPTIMIZATION

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Within the past decade, the field of data-driven mathematics has progressively gained in importance due to advances in data analysis, artificial intelligence and, foremost, in data availability. Methods like machine learning (ML) are becoming more powerful, enabling systems and machines to act and to learn increasingly autonomously. Here, neural networks (NNs) are one of the most dominant ML models. In the context of mobility applications, the interest in self-driving cars and intelligent traffic management systems is rapidly growing, as well as the demand for efficient controllers for such systems. The training of a NN for such applications usually poses a non-convex optimization problem with an objective function that has numerous local extrema. Consequently, using gradient-based local optimization algorithms, as it is typically done for NN training, the training procedure often converges to a specific local minima. The latter, in turn, strongly depends on the choice of the initial values for the optimization loop - in the NN training context, these are initial values for weights and biases of the NN. Thus, the training process is non-robust in a sense that small changes in the initial values may lead to substantially different results. This effect makes a systematic analysis of the influence of structural network parameters and algorithmic parameters (often called hyper-parameters) very challenging. Optimizing those parameters is very difficult, if even possible. In classical optimization, however, so-called particle swarm optimization techniques (PSO) are known as a tool for escaping local minima in non-convex optimization processes [1].

In this work, we show how the combination of such a PSO approach with conventional gradient-based NN training can substantially increase training robustness of recurrent neural networks. We use a slightly modified version of a classical PSO approach to escape local minima in NN training and, thus, to reduce the impact of (randomly chosen) initial weights and biases. In this context, classic recurrent NNs as well as echo state networks are investigated. Moreover, we demonstrate the applicability and the quality of the proposed approach by applying it to two examples from vehicle control. In the first example, a lateral dynamics model of a truck-trailer combination is considered. Here, the objective is to determine a NN-based optimal steering controller. In the second example, a NN needs to be trained to optimally control a virtual platoon. For both cases, we show how a PSO-based training process can significantly improve the robustness and the quality of the achieved training results, which enables analyzing and optimizing structural NN parameters for the corresponding application.

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ROAD PROFILE IDENTIFICATION VIA ITERATIVE LEARNING CONTROL

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In this contribution, we consider inverse tracking problems in vehicle engineering. Hereby, the goal is to compute input or excitation signals for dynamic systems in order to reproduce measured output reference data. For instance, such input signals are needed for simulations of vehicular (sub-)systems. In particular, the quarter-car (suspension) model requires the road profile as input to simulate the displacement of the lower and upper body masses, velocities or accelerations of those and resulting forces. Moreover, these input quantities are also often necessary to control real test-rigs in the laboratory. Mathematically, this task – identifying input signals based on given reference outputs – is an inverse problem that can be solved with approaches from optimal control theory [1,2].

We present the state-of-the-art approach to solve such inverse problems in vehicle engineering: the iterative learning control (ILC) method [2]. This methodology is widely used in industrial applications, especially in durability testing. In the ILC approach, first a linear surrogate model of the system is estimated based on specifically generated input-output data pairs using spectral methods. Then, the inverse problem is solved via a Newton-like iteration procedure that makes use of the surrogate model and computes the inverse of the latter to derive input updates in each iteration step.

We apply and demonstrate the presented methodological approach in a framework for identifying road profiles based on (easily accessible) measurement data on a three axle trailer. Based on a full vehicle model of the trailer, the corresponding control quantities, i.e. left and right vertical road profile, are determined to reproduce the measured vertical axle accelerations, spring displacements or wheel forces.

Acknowledgments Parts of the work presented in this contribution have been developed within the project IdenT (Identifikation dynamik- und sicherheitsrelevanter Trailerzustände für automatisiert fahrende Lastkraftwagen) [3], which is funded by the Federal Ministry for Economy and Climate Protection based on a resolution of the German Bundestag.

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RESOURCE CONSCIOUS FAULT CLASSIFIERS

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As condition monitoring of systems continues to grow in both complexity and application an overabundance of data is amassed [1]. Computational capabilities are unable to keep abreast of the subsequent processing requirements. Thus, a means of establishing computable prognostic models to accurately reflect process condition, whilst alleviating computational burdens, is essential. This is achievable by quantifying a parameter' s explanatory power and restricting input of redundant information to modelling algorithms.

This presentation will focus on methods of reducing input parameter volume without sacrificing model efficiency. Assessing underlying parameter variances to facilitate input variable selection whilst maintaining parameter characteristics. A number of approaches will be discussed including variable clustering to reorganise the harmonics of common diagnostic features into a smaller number of heterogeneous groups representatives from each selected to reflect conditions with minimal information redundancy. Furthermore, generic parameter capabilities evidenced through confirmatory factor analysis enable parameters with superior deterministic power to be identified alongside complimentary, uncorrelated, variables. Particularly, variables with little explanatory capacity can be eliminated and lead to further variable reductions. Applications demonstrated in predictive maintenance of industrial rotating machinery [2].

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CT 16

	Friday
Room	CR 106
10:40-11:05	Haolin Yang
11:05-11:30	Michael Kniely
11:30-11:55	Manuel Ettmuller
11:55-12:20	William Lee

INDUSTRIAL MELT SPINNING WITH TWO-WAY COUPLED AIR FLOW INCLUDING CRYSTALLIZATION AND RADIAL EFFECTS

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

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

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

A THERMODYNAMICALLY CORRECT FRAMEWORK FOR ELECTRO–ENERGY–REACTION–DIFFUSION SYSTEMS

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We consider a thermodynamically consistent formulation of reaction–diffusion systems modeling the evolution of a mixture of charged species. This approach covers, in particular, a large class of (inorganic) semiconductor-type models. Here, thermodynamical consistency refers to the validity of fundamental conservation laws and the production of entropy. This is achieved by a gradient flow system in Onsager form for the concentrations and the internal energy coupled to Poisson's equation for the electrostatic potential.

We will first focus on the structure of the Onsager operator and the incorporation of the electrostatic potential within its diffusive component. Similarities and differences to other temperature-dependent semiconductor-type models shall be addressed as well. This concerns, e.g., the choice of independent variables, different entropy functionals, and admissible mobility matrices.

One of the goals of this project is the construction of global solutions (either in a weak or a renormalized sense) to an appropriate class of electro–energy–reaction–diffusion systems. First results in this direction will be presented, while open problems shall be discussed as well. This project is joint work together with Alexander Mielke.

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UNEVEN EXTRACTION IN COFFEE BREWING

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Coffee is a drink made by dissolving the soluble parts of ground, roast coffee beans in water [1]. In espresso coffee this is done at high temperatures and pressures. It seems obvious that grinding coffee more finely will lead to more coffee being extracted. However, a recent experiment showed that, beyond a cutoff point grinding coffee more finely results in lower extraction [2]. One possible explanation for this is that fine grinding promotes uneven extraction in the coffee bed. To explore this a low dimensional model in which there are two possible pathways for flow and coffee extraction is derived and analysed [3]. This model shows that, below a critical grind size, there is decreasing extraction with decreasing grind size as is seen experimentally. In the model this is due to a complicated interplay between an initial imbalance in the porosities and permeabilities of the two pathways which is increased by flow and extraction, leading to the complete extraction of all soluble coffee from one pathway.

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MATHEMATICAL MODELLING OF LUBRICATED FLOWS

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Motivated by geophysical, industrial and physiological applications, we develop a mathematical model for the flow of a thin film of viscous fluid spreading over a lubricated substrate, which we examine using asymptotic and numerical methods. We apply lubrication theory to model the flow as a thin film of viscous fluid spreading over a horizontal substrate that is pre-wetted with another layer of fluid. In our modelling, we assume that the effects of inertia and surface tension are negligible. By performing an asymptotic analysis, we characterise a frontal singularity occurring at the intrusion front, and compare our asymptotic solutions against full numerical solutions for the thicknesses of the two layers of fluid. We find conditions under which the flow is self similar and we examine similarity solutions across a number of regimes in terms of key dimensionless parameters, including the ratio of the viscosities of the two layers of fluid, the dimensionless density difference between them, and the dimensionless source fluxes. The dynamics range from those of viscous gravity currents propagating over a deep layer to those lubricated by a thin, pre-wetting film. Depending on the viscosity ratio, the behaviour of the intruding layer ranges from that of a thin coating film, which exerts negligible traction on the lubricated substrate, to a very viscous gravity current spreading over a low-viscosity layer. Large differences in the densities of the two fluids yield flows similar to single-layer viscous gravity currents spreading over a rigid, mobile substrate.

CT 17

	Friday
Room	CR 10 B
15:30-15:55	Nataliya Togobytska
15:55-16:20	Zsolt Vizi
16:20-16:45	Nhat Tan Le

PRICING FINITE-MATURITY MARGIN CALL STOCK LOANS

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This paper examines the pricing issue of margin-call stock loans with finite maturities. In particular, using a Fourier Sine transform method, we reduce the partial differential equation governing the price of a margin call stock loan into an ordinary differential equation, the solution of which can be easily found (in the Fourier space) and analytically inverted into the original space. As a result, we can derive the "early exit premium representation" for the margin-call stock loans and show that a finite maturity margin call stock loan can be considered as an American-style down-and-out call with a time-dependent strike price and barrier. On top of that, we can break the pricing problem of margin call stock loans into two simple steps: 1) finding the optimal exit prices and 2) calculating the value of margin call stock loans. Our numerical results appear to fit very well with those obtained from the pertinent literature.

Keywords: Margin call stock loan, Fourier transform, Integral equation, Optimal exercise boundary, American-style down-and-out call options.

ADAPTIVE SEGMENTED REGRESSION FOR THE MODELING OF TEMPERATURE-DEPENDENT MATERIAL PROPERTIES

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This paper presents a mathematical approach for the modeling of the physical properties of steel slag. Steel slag is an industrial by-product discharged from the steelmaking process. It is generated in large quantities and has the potential to become a significant source of landfill waste and pollution. Technology has come up to recycle and reuse reprocessed, granulated slag as a sustainable construction material. It is important to study the physical properties of slag melts and the factors that affect them. The modelling of temperature-dependent electrical conductivity and viscosity of slag melts is based on an approximation by peacewise linear regression in the temperature ranges defined by an expert [1,2]. We propose a genetic algorithm for the derivative-free optimization of breakpoints in segmented regression to increase the reliability of the modeling results. The results obtained are of practical importance when selecting rational slags for different metallurgical processes.

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MATHEMATICAL METHODS FOR DATA-DRIVEN APPROACHES IN WATER MANAGEMENT

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The water management directorates in Hungary manage the professional duties of tasks like coordinating flood control and water management programs, and organizing flood damage related activities. Since manual recording of water level data was upgraded with installation of measurement devices at the gauging stations, a large amount of data is created on a daily basis, but only a relatively small fraction of it is used on the operational level of the work. In the collaboration of University of Szeged, Water Management Directorate of Alsó-Tisza and Smart Software Consulting Ltd., several data-related problems were considered for improving the currently used tools and methodologies in the water management area in the last two years.

In this talk, we present the results of the ongoing R&D activities covering two main topics. On one hand, a mathematical framework is introduced for formally analyzing flood wave along the river Tisza representing the temporal behavior of the flood waves as a special graph. The software developed in a pilot project allows the professionals to investigate the effect of river control activities and to understand better the differences between different sections of the river. On the other hand, we show a data-driven model developed for predicting water level and a detailed evaluation setting to explore strengths and weaknesses of the model and to enable pragmatic tools to compare forecasting models. Since existing approaches use fluid dynamics or statistical methodolgy, clear understanding about the limitations in the models might lead to apply ensembling techniques, which could combine expert knowledge and information extracted from the underlying data.

CT 18

	Tuesday
Room	CR 115
17:20-17:45	Dana Mackey
17:45-18:10	Jack Lyons
18:10-18:35	Néstor García-Chan
18:35-19:00	Olena Andrusenko

MODELING OF DRILL STRING BUCKLING IN 3D CURVILINEAR BORE-HOLES

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This paper deals with the problem of simulating the regimes of drilling deep curvilinear bore-holes with prescribed imperfect geometrical trajectories of their axial lines. On the basis of the theory of curvilinear flexible elastic rods, the 3D "stiff-string" drag and torque model of the drill string bending and the appropriate software are elaborated for the simulation of the tripping in and out regimes and drilling operations [1]. It is shown that the contact and friction forces can be calculated and regulated. The elaborated software can be used for the emergency situations prognostication and their exclusion at the stages of the drilling process design and realization [2].

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URBAN HEAT ISLAND DYNAMICS IN AN URBAN-RURAL POROUS DOMAIN, NUMERICAL METHODOLOGY AND SIMULATION

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Heat transfer and fluid dynamics modeling in porous media is a widely explored topic in physics and applied mathematics involving advanced numerical methods to address its non-linear nature [1]. One exciting application has been the urban heat island (UHI) numerical simulation [2]. The UHI is a negative consequence of the increasing urbanization in cities being defined as the presence of warm temperatures inside the urban canopy with respect to the colder surroundings. Furthermore, interesting phenomena occur in the UHI context, the city turns from a heat island during the day to a cold island at night with respect to its rural surrounding, and the wind gusts as a factor to relieve the UHI intensity. Thus, in contrast with [2] the key elements proposed in this work are: a 2d horizontal urban-rural domain whose variable porosity has a Gaussian distribution centered in the city downtown, and a non-stationary Darcy-Forchheimer-Brinkman model to simulate flow in a porous media combined with an air-surface-soil heat transfer model. In regards to the numerical resolution of the model, a classical numerical methodology based on finite elements of Lagrange P_1 type combined with explicit and implicit time marching schemes has shown to be good enough to reach high-quality numerical solutions. Several numerical tests have been performed on a domain inspired in the Metropolitan Area of Guadalajara (Mexico), in which, not only the temperature inversion was reproduced but also the simulation of UHI overturn by a strong blowing wind.

Acknowledgments The first author is grateful for the support of CONACyT-Ciencia de Frontera (grant 217556).

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MODELLING THE EFFECT OF ZEOLITE DOPANTS ON OPTICAL PATTERNING OF PHOTOPOLYMERS

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This talk introduces a mathematical model for holographic grating formation in an acrylamide based photopolymer containing zeolite nano-dopants. A hologram is essentially a recording of an interference pattern created by an object beam and a reference beam in a photosensitive material through changes in its optical properties, and optical photopatterning has applications in areas such as optical elements and sensors, security holograms and data storage. The subject of this study are phase holograms, which are recorded as spatial variation in the refractive index of the photosensitive material.

The model consists of partial differential equations describing physical processes such as mass transport of various photopolymer constituents, photopolymerisation and cross-linking of long polymer chains, [1]. Our current research emphasis is on how the addition of the zeolite dopants impacts on the dynamics of the system and the resulting refractive index modulation through nanoparticle redistribution, which affects the diffusion of all other components, and light scattering. Both modelling results and experimental data consistently show significant advantages of doped materials, such as increases in diffraction efficiency and grating strength and reduced photopolymerisation-induced shrinkage, [2]. We also briefly discuss holographic sensors, which are analytic devices that contain a holographic grating embedded in a functionalised photopolymer, which can change their optical properties when exposed to target analytes.

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MODELLING THE FORMATION OF SLANTED HOLOGRAPHIC GRATINGS IN HYBRID PHOTOPOLYMER MEDIA

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There is growing commercial interest in photopolymers as a recording media for holographic applications. The self-processing nature, low production costs and wide dynamic range make them an ideal candidate for the fabrication of holographic sensors, diffractive optical elements and data storage. One metric for the performance of such applications is a high diffraction efficiency which is largely determined by refractive index modulation (Δn). One technique used to increase Δn is the addition of inorganic nanoparticles to the recording matrix; spatial redistribution of inert nanoparticles during recording results in a positive contribution to Δn. Existing mathematical models for holographic grating formation do not account for nanoparticle redistribution. Furthermore, the existing models have restricted analysis to a single spatial dimension and thus cannot predict how the thickness of the recording medium is significant in determining Δn observed in studies of holographic recording in photopolymer media [1]; the formation of slanted holographic gratings also cannot be simulated with existing models. This proposed talk for ECMI 2023 will cover how the existing mathematical models have been augmented to account for photochemical reactions and mass transport in two spatial dimensions, redistribution of inorganic nanoparticles and photon scattering. Another metric for the performance of holographic recording media is low photopolymerization induced material shrinkage. Earlier studies have found that the concentration of inorganic nanoparticles [2] and thickness of the recording medium [1] have shown to be a significant influence on shrinkage. As already mentioned, existing mathematical models do not account for nanoparticle doping nor the finite depth of the recording medium. This proposed talk for ECMI 2023 will also discuss how a new mathematical model can predict the observed shrinkage in slanted holographic gratings recorded in hybrid photopolymer media.

Acknowledgments The authors are grateful for the support of the Irish Research Council (grant GOIPG/2021/214).

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Part VII

Industry Day

APPLICATION OF STOCHASTIC PROCESSES FOR MODELLING MARKET RISK FACTORS IN A MINING COMPANY

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In order to properly manage market risk, mining companies have to forecast potential price scenarios for main market risk factors. Stochastic modelling stands out among forecasting methods due to the fact that they do not assume a single forecasting path but rather takes into account inbuilt randomness of the process and large range of potential outcomes. Commonly used stochastic models usually does not reflect market data characteristics like heteroscedasticity, heavy tails, regime switching or stability of interdependence between market risk factors. The presentation includes models addressing these characteristics.

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HOW MATH IS HELPING PEOPLE AND BUSINESS TO PROSPER

Adam Ocharski

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We will explore the role that mathematics plays in financial industry and the profound role that its application has on organisational structure of Santander, talent management, as well as technology development. What future holds for union on financial industry and science? What is the meaning for our customer? Can we succeed without it?

SUN CABLE AND RESEARCH INITATIVES

Jakub Tomczyk

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Creating large pieces of renewable infrastructure requires interactive interfaces between many disciplines. In particular, replicating the connectivity of European energy systems within Southeast Asia requires a range of technological innovations and development of region specific know-how. In this talk, I will discuss research initiatives from PV yield modelling through subsea cables modelling to system level optimisation, which should support the decision-making processes in renewable energy developers of the future. Also, I will outline potential research directions and how they can benefit the future interconnected electricity grid in Asia.

Practitioner View on Derivatives Pricing

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Pricing derivatives is a vital component for functioning on the money markets. This talk provides an overview on the financial-engineering toolkit highlighting the practical aspects. The starting point of this talk aims at presenting how to model stock prices [1]. Then the price of a derivative is determined by the cost of its hedging strategy. It is stressed that the pricing framework builds on risk neutral measure that only works if the traders hedge their risks [2]. Second part of the talk is dedicated to the risk management associated with derivatives and its outlook.

References

1. M. Baxter, A. Rennie, *Financial Calculus*, Cambridge University Press, 1996
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WORLD OF SWAPTIONS - PRICING, CALIBRATION, VOLATILITY

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Understanding of Vanilla Interest Rate Swaps and European Swaptions is a fundamental aspect in the pricing and hedging interest rate derivatives. This talk aims at highlighting the motivations to trade these instruments as well as describes market standards pertaining to the fair swap rate definition and the swaption volatility surface and cube. Basic theoretical foundations underlying valuation of swaptions will also be presented, i.e. Black 76 model, which is a fixed income counterpart of the renowned Black-Scholes model [1]. Moreover, as an extension to the Black-Scholes model, foundations of Stochastic Alpha Beta Rho model (SABR), with calibration results will be presented [2]. Finally, most recent changes that take place in financial markets regarding LIBOR decommission will be discussed.

References

1. D. D. McInerney, T. Zastawniak, Stochastic Interest Rates, *Cambridge University Press*, 104 pp., 2015
2. C. Crispoldi, G. Wigger and P. Larkin, SABR and SABR LIBOR Market Models in Practise With Examples Implemted in Python, Second Edition. *Palgrave Macmillan*, 2015. 42 pp.

EARTH IMAGERY AND PROCESSING IN NEW SPACE INDUSTRY

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SatRev, established in 2016, aims to democratize space and integrate Earth Observation capabilities into the innovative CubeSat standard of nanosatellites. In 2019, our first satellite, "Światowid," was launched from the ISS, demonstrating SatRev's Imagery instrument capabilities and paving the way for a Real-Time Earth Observation Constellation.

Fast forward to 2023, SatRev has successfully deployed 11 satellites into orbit, including 5 of our standard STORK 3U CubeSats, equipped with our in-house developed Camera. Operating at the forefront of scientific and New Space endeavours, our workload envelops Earth imagery processing and utilization, imaging instrument development, and in-orbit demonstrations for customer-conceived space components.

In Earth Imagery processing, we leverage the power of artificial neural networks and deep learning models, specializing in semantic segmentation. This intricate task precisely partitions complex images into distinct regions based on semantic content. Our expertise extends to Imaging Instrumentation, where we utilize our deep understanding of optics, materials science, systems engineering, and standard sequential ray tracing techniques. This comprehensive knowledge allows us to conceive and fabricate state-of-the-art telescopes that push the boundaries of observational capabilities.

Furthermore, SatRev plays an instrumental role in facilitating the demonstration of customer-developed space components in the challenging environment of outer space. We subject these components to rigorous tests and evaluations, both in simulated and real-world conditions, providing comprehensive support throughout the development stages of our customers' solutions.

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