2nd International Conference on Simulation Technology

Stuttgart
26 – 28 March 2018
Changes and Editorial Mistakes (16 March 2018)

Editorial Mistakes

1. The Keynote lecture of Omar Ghattas takes place from 2:00 to 2:45 pm on Wednesday, 28 March 2018. Unfortunately, on page 38 in the printed version it states a different time.

2. The Keynote lecture of Michael Ortiz takes place from 2:45 to 3:30 pm on Wednesday, 28 March 2018. Unfortunately, on page 38 in the printed version it states a different time.

Changes

1. There will be an additional poster for PN 1 with the number PP1.000 (page 58)
   
   A variational framework for distance-minimizing data-driven computing method
   Lu Trong Khiem Nguyen, Matthias Rambausek, Marc-André Keip


4. The poster title of poster PP 4.046 (page 81) by Ewa Anna Oprzeska-Zingrebe and Jens Smiatek has changed. The new title is:

   Preferential binding of urea to single-stranded DNA structures: a MD simulation study

5. The poster title of poster PP4.080 (page 87) by Maria Hammer and Syn Schmitt has changed. The new title is:

   SimWalk – a simulation framework and testbed for digital human walking
Programme for the

2nd International Conference on Simulation Technology
Content

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Welcome Address
From 26th to 28th March 2018, Stuttgart will host simulation technology’s leading researchers for the 2nd International Conference on Simulation Technology (SimTech 2018).

The conference agenda covers numerous topics related to the field of simulation technology, such as advanced mechanics, molecular simulations, numerical mathematics, and interactive visualization, to name just a few.

SimTech 2018 is a major platform for promoting exchange amongst representatives of the international community in a variety of fields, bringing together mathematicians and biochemists, engineers and chemists, computer scientists and sociologists, physicists and philosophers. In keynote lectures, renowned scientists present the latest ideas from the world of simulation technology.

With the multi-disciplinary environment at SimTech 2018, we continue to advance towards our goal at the Stuttgart Cluster of Excellence in Simulation Technology: developing simulation technology from isolated numerical approaches to an integrative systems science.

Our sincere thanks go to all participants for their valuable contributions. We are proud to welcome you in Stuttgart and trust that this conference will be an enriching scientific and personal experience.

Stuttgart, March 2018

Professor Wolfgang Ehlers
Spokesperson and Executive Director of the Cluster of Excellence in Simulation Technology
Team
GENERAL CHAIRS

- Frank Allgöwer, Institute for Systems Theory and Automatic Control
- Wolfgang Ehlers, Institute of Applied Mechanics (CE)
- Thomas Ertl, Institute for Visualization and Interactive Systems
- Rainer Helmig, Institute for Modelling Hydraulic and Environmental Systems
- Christian Rohde, Institute of Applied Analysis and Numerical Simulation

LOCAL SCIENTIFIC COMMITTEE

- Christian Holm, Institute for Computation Physics
- Marc-André Keip, Institute of Applied Mechanics (CE)
- Frank Lehmann, Institute for Construction Materials
- Guido Schneider, Institute of Analysis, Dynamics and Modeling
- Miriam Mehl, Institute of Parallel and Distributed Systems
- Michael Resch, Institute of High Performance Computing
- Albrecht Schmidt, Institute for Visualization and Interactive Systems
- Meike Tielbein, Institute for Diversity Studies in Engineering
- Wolfgang Weimer-Jehle, Center for Interdisciplinary Risk and Innovation Studies
- Hans-Joachim Werner, Institute for Theoretical Chemistry

ORGANISING COMMITTEE

- Ashish Bhatt, Institute of Applied Analysis and Numerical Simulation
- Katrin Bogisch, SimTech
- Felix Fritzen, Institute of Applied Mechanics
- Dieter Höhn, Institute of Thermodynamics and Thermal Process Engineering
- Tobias Köppl, Institute for Modelling Hydraulic and Environmental Systems
- Nicole Radde, Institute for Systems Theory and Automatic Control
- Marianne Richter, SimTech
- Gabriele Santin, Institute of Applied Analysis and Numerical Simulation
- Malte von Scheven, Institute for Structural Mechanics
- Sabine Sämisch, SimTech
- Barbara Teutsch, SimTech
- Arndt Wagner, Institute of Applied Mechanics (CE)
- Reiner Dietz, SimTech
- Tatjana Ahle, SimTech
- Regina Strammer, SimTech
General Information
**COFFEE BREAKS**

During the coffee breaks coffee, tea, soft drinks, snacks and fresh fruit will be served on Level -1.

**CONFERENCE SECRETARIAT/INFO POINT**

If you need assistance or have any questions, please contact the conference secretariat at the info point in the main hall on the ground floor. There you get information about the technical and social programme of the conference as well as public transport, WLAN and places of interest in Stuttgart.

**CONFERENCE STAFF**

Members of the conference team are present at the conference secretariat and in all lecture rooms. You will recognise them by the orange shirts and orange lanyards.

**INTERNET ACCESS**

The University of Stuttgart provides free wireless internet access to all participants. You can choose between two kinds of authentication:

1. **Eduroam**
   
The University of Stuttgart is part of the Eduroam initiative. The Eduroam network is available in most parts of the building and can be accessed with the account of your home institution, if your home institution also takes part in Eduroam.

2. **Conference Network**
   
The conference network (SSID: konferenz) can be used with WPA2 encryption. The passwords change from day to day:
   
<table>
<thead>
<tr>
<th>Day</th>
<th>Password</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monday, 26 March 2018</td>
<td>052-630-173-149</td>
</tr>
<tr>
<td>Tuesday, 27 March 2018</td>
<td>902-487-378-233</td>
</tr>
<tr>
<td>Wednesday, 28 March 2018</td>
<td>730-124-279-130</td>
</tr>
</tbody>
</table>

By using this internet access, you agree with the terms of use for digital data processing and communication technology at the University of Stuttgart.

**LUNCH**

Lunch will be served from 12:00 to 2:00 pm at the “Mensa” of the University of Stuttgart or at the cafeteria “Contrast”. The lunch includes a starter or a dessert, a main course including side dishes and one drink. Make sure you have your lunch voucher with you.
REGISTRATION
In order to avoid unnecessary waiting time and to ensure the planned schedule, registration already starts at 8:30am on Monday morning. The registration or info desk can be found at Pfaffenwaldring 47.

TAXI
Taxi can be ordered at the conference secretariat or directly at Taxi-Auto-Zentrale via +49 (0)711 5510 000.

TOURIST INFORMATION
The tourist information is located next to the main station in the Königstraße, which is the main shopping street in Stuttgart.

WARDROBE & LUGGAGE
On the ground floor you can leave your jackets and luggage in room 47.06. The room is situated next to the entrance and info point.

Opening hours are:
Monday, 26 March 8:00 am to 6:00 pm and 9:00 pm to 9:30 pm
Tuesday, 27 March 8:00 am to 6:00 pm
Wednesday, 28 March 8:00 am to 5:00 pm
Venue Map
The University of Stuttgart will provide the venue for SimTech 2018. The site is very conveniently situated. The events for SimTech 2018 can be accessed by rail from Stuttgart Airport in only 15 minutes.
How to get there

1. From Stuttgart Airport ("Flughafen")

**Local train (S-Bahn):** Please follow the sign in the arrival hall. For the ride to the conference venue you require a ticket for two zones (single ride € 2.90) which can be bought at the ticket machines at the entrance of the train station.

Please take lines S2 (direction “Schorndorf”) or S3 (direction “Backnang”). The ride will take about 16 minutes to the station “Universität”. Leave the train station via the exit in the direction of travel (direction “Universitätszentrum”) and follow the conference signs.

**Taxi:** Taxis are located right in front of the arrival hall. The taxi ride to the conference venue takes about 15 to 20 minutes (approx. € 25 to 30).

2. From Stuttgart Main Station ("Hauptbahnhof")

**Local train (S-Bahn):** Please follow the sign in the arrival hall. For the ride to the conference venue you require a ticket for two zones (single ride € 2.90) which can be bought at the ticket machines at the entrance of the train station.

Please take lines S2, S2 or S3 from platform 101 (underground). The ride will take about 11 minutes to the station “Universität”. Leave the train station via the exit opposite to the direction of travel (direction “Universitätszentrum”) and follow the conference signs.

**Taxi:** Taxis are located right in front of the arrival hall. The taxi ride to the conference venue takes about 15 to 20 minutes (approx. € 25 to 30).
3. By Car

![Map showing the route from Pfaffenwaldring to the conference venue.]

4. Parking

There are free parking lots next to the conference venue. From the street Pfaffenwaldring follow the signs Pfaffenwaldring 11+13+15. You will find parking lots to left of the road. The conference venue is located at the far end of the parking lots.

![Map showing public transport from the main station to the conference venue.]
Conference Schedule
<table>
<thead>
<tr>
<th>Time</th>
<th>Monday, March 26th</th>
<th>Tuesday, March 27th</th>
<th>Wednesday, March 28th</th>
</tr>
</thead>
<tbody>
<tr>
<td>09:00 – 10:30</td>
<td>From Local Modification to Global Effects in Finite Element Flow Simulation (Barbara Wohlmuth)</td>
<td>Surviving the Data Deluge: A Systems and Control Perspective (Mario Sznaier)</td>
<td>Atomistic Molecular Simulations for Process Engineering: Methods, Tools and Results (Jadran Vrabec)</td>
</tr>
<tr>
<td>10:30 – 11:00</td>
<td>Opening</td>
<td>Coffee Break</td>
<td>Coffee Break</td>
</tr>
<tr>
<td>11:00 – 12:30</td>
<td>Neuromechanics – Perspectives, Challenges, and Opportunities (Ellen Kuhl)</td>
<td>Mini Symposium 2</td>
<td>Optimization by Simulation: Heuristics and Certificates (Marco Campi)</td>
</tr>
<tr>
<td></td>
<td>Citius, altius, fortes! (Hans-Joachim Bungartz)</td>
<td>Mini Symposium 6</td>
<td>Next Generation Physical Analytics (Nigel Davies)</td>
</tr>
<tr>
<td>12:30 – 14:00</td>
<td>Lunch Break</td>
<td>Lunch Break</td>
<td>Lunch Break</td>
</tr>
<tr>
<td>14:00 – 15:30</td>
<td>Mini Symposium 1</td>
<td>Poster Session</td>
<td>Optimization Under Uncertainty for Complex PDE Models in High Dimensions (Omar Ghattas)</td>
</tr>
<tr>
<td></td>
<td>Mini Symposium 3</td>
<td></td>
<td>Data-Driven Computing (Michael Ortiz)</td>
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<tr>
<td></td>
<td>Mini Symposium 4</td>
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<tr>
<td></td>
<td>Mini Symposium 5</td>
<td></td>
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</tr>
<tr>
<td>15:30 – 16:00</td>
<td>Coffee Break</td>
<td>Coffee Break</td>
<td>Poster Award and Closing</td>
</tr>
<tr>
<td>16:00 – 17:30</td>
<td>Simulation of Complex Social Phenomena: Concepts and Challenges (Ortwin Renn)</td>
<td>Mesoscopic Modelling of Active Materials: Selfassembly and Emergent Properties (Ignacio Pagonabarraga)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>On Using System Dynamics to Build Adaptive Capacity with Small-scale Farmers in sub-Saharan Africa (Birgit Kopainsky)</td>
<td>Deep Neural Networks in Simulation Science (Jan Hesthaven)</td>
<td></td>
</tr>
<tr>
<td></td>
<td>Get Together</td>
<td>Conference Dinner</td>
<td></td>
</tr>
</tbody>
</table>
08:30 am – 10:00 am  
Registration  
Pfaffenwaldring 47

10:00 am – 11:00 am  
Opening  
Pfaffenwaldring 47, 47.03

11:00 am – 11:45 am  
Keynote Lecture  
NEUROMECHANICS – PERSPECTIVES, CHALLENGES, AND OPPORTUNITIES  
Ellen Kuhl | V 47.03

11:45 am – 12:30 pm  
Keynote Lecture  
CITIUS, ALTIUS, FORTIUS!  
Hans-Joachim Bungartz | V 47.03

12:30 pm – 2:00 pm  
Lunch Break

2:00 pm – 3:30 pm  
Mini Symposia

<table>
<thead>
<tr>
<th>Mini Symposium 1</th>
<th>Mini Symposium 3</th>
<th>Mini Symposium 4</th>
<th>Multi-phase &amp; Multi-Physics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Multi-scale and multi-field</td>
<td>Dynamic Systems</td>
<td>Biomechanics &amp; systems biology</td>
<td>Multi-phase &amp; Multi-Physics</td>
</tr>
<tr>
<td>Room: 47.05</td>
<td>Room: 9.01</td>
<td>Room: 47.03</td>
<td>Room: 7.01</td>
</tr>
<tr>
<td>Miguel Bessa (30’)</td>
<td>Anne Romer</td>
<td>Jan Haasenauer</td>
<td>Isabell Faille</td>
</tr>
<tr>
<td></td>
<td>Tobias Holicki</td>
<td></td>
<td>Roland Masson Unice</td>
</tr>
<tr>
<td></td>
<td>Andreas Hoffmann</td>
<td>Nicole Radde</td>
<td>Michael Dumbser</td>
</tr>
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<td></td>
<td>Philip Tempel</td>
<td>Syn Schmitt</td>
<td>Martin Schneider</td>
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<tr>
<td></td>
<td>Andreas Schmidt</td>
<td>Tim Ricken</td>
<td>Guang Yang</td>
</tr>
</tbody>
</table>

3:30 pm – 4:00 pm  
Coffee Break

4:00 pm – 4.45 pm  
Keynote Lecture  
SIMULATION OF COMPLEX SOCIAL PHENOMENA: CONCEPTS AND CHALLENGES  
Ortwin Renn | V 47.03

4:45 pm – 5:30 pm  
Keynote Lecture  
ON USING DYNAMICS TO BUILD ADAPTIVE CAPACITY WITH SMALL-SCALE FARMERS IN SUB-SAHARAN AFRICA  
Birgit Kopainsky | V 47.03

6:30 pm – 9:30 pm  
Get Together  
Pfaffenwaldring 47
Tuesday, 27 March 2018

9:00 am – 9:45 am
Keynote Lecture
FROM LOCAL MODIFICATION TO GLOBAL EFFECTS IN FINITE ELEMENT FLOW SIMULATION
Barbara Wohlmuth | V 47.03

9:45 am – 10:30 am
Keynote Lecture
OPENSPACE – VISUALIZING THE UNIVERSE
Anders Ynnerman | V 47.03

10:30 am – 11:00 am
Coffee Break

11:00 am – 12:30 pm
Mini Symposia

<table>
<thead>
<tr>
<th>Mini Symposium 2</th>
<th>Mini Symposium 6</th>
<th>Mini Symposium 7</th>
</tr>
</thead>
<tbody>
<tr>
<td>High performance simulations</td>
<td>Cyber infrastructure</td>
<td>Reflexion &amp; Contextualisation</td>
</tr>
<tr>
<td>Room: 47.03</td>
<td>Room: 9.01</td>
<td>Room: 47.05</td>
</tr>
<tr>
<td>Tristan Bereau</td>
<td>Peter Reimann</td>
<td>Florian Kappmeier</td>
</tr>
<tr>
<td>Philipp Marquetand</td>
<td>Michael Hahn</td>
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<tr>
<td>Michael Lahner</td>
<td>Christoph Dibak</td>
<td></td>
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<tr>
<td>Alexander Denzel</td>
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</table>

12:30 pm – 2:00 pm
Lunch Break

2:00 pm – 3:30 pm
Poster Session
Pfaffenwaldring 47, Lower and Ground Floor

3:30 pm – 4:00 pm
Coffee Break

4:00 pm – 4:45 pm
Keynote Lecture
MESOSCOPIC MODELLING OF ACTIVE MATERIALS: SELFASSEMBLY AND EMERGENT PROPERTIES
Ignacio Pagonabarraga | V 47.03

4:45 pm – 5:30 pm
Keynote Lecture
DEEP NEURAL NETWORKS IN SIMULATION SCIENCE
Jan Hesthaven | V 47.03

6:00 pm
Bus transfer & Exhibition
Mercedes-Benz Museum, Stuttgart

8:00 pm – 11:00 pm
Conference Dinner
Mercedes-Benz Museum, Stuttgart
9:00 am – 9:45 am
Keynote Lecture
SURVIVING THE DATA DELUGE: A SYSTEMS AND CONTROL PERSPECTIVE
Mario Sznaier | V 47.03

9:45 am – 10:30 am
Keynote Lecture
ATOMISTIC MOLECULAR SIMULATIONS FOR PROECESS ENGINEERING: METHODS, TOOLS AND RESULTS
Jadran Vrabec | V 47.03

10:30 am – 11:00 am
Coffee Break

11:00 am – 11:45 am
Keynote Lecture
OPTIMIZATION BY SIMULATION: HEURISTIC AND CERTIFICATES
Marco Campi | V 47.03

11:45 am – 12:30 pm
Keynote Lecture
NEXT GENERATION PHYSICAL ANALYTICS
Nigel Davies | V 47.03

12:30 pm – 2:00 pm
Lunch Break

2:00 pm – 2:45 pm
Keynote Lecture
OPTIMIZATION UNDER UNCERTAINTY FOR COMPLEX PDE MODELS IN HIGH DIMENSIONS
Omar Ghattas | V 47.03

2:45 pm – 3:30 pm
Keynote Lecture
DATA-DRIVEN COMPUTING
Michael Ortiz | V 47.03

3:30 pm – 4:00 pm
Poster Award and Closing
V 47.03
Keynote Lectures and Speakers
Arguably, the brain is the most complex organ of our body, and – at the same time – the least well understood. The fields of neuroscience, neurobiology, and neuroimaging have seen tremendous progress throughout the past two decades; yet, the field of neuromechanics remains underappreciated and poorly understood. Here, we discuss the importance of neuromechanics in integrating knowledge across the disciplines and scales, from individual neurons to the brain as a whole. We show that mechanical stretch, strain, and stress play a critical role in modulating the structure and function of the human brain. Using the nonlinear field theories of mechanics, we illustrate two phenomena, which are tightly regulated by mechanical factors: neurodevelopment, the formation of the brain, and neurosurgery, the mechanical manipulation of the brain. We hope that this presentation will inspire discussion around the mechanics of the brain with potential impact in preventing, diagnosing, and treating neurological disorders.

Ellen Kuhl is a Professor of Mechanical Engineering and Bioengineering at Stanford University. She received her PhD from the University of Stuttgart in 2000 and her Habilitation from the University of Kaiserslautern in 2004. Her area of expertise is Living Matter Physics, the creation of theoretical and computational models to predict the behavior of living systems. Ellen is the Vice Chair of the U.S. National Committee on Biomechanics, a Fellow of the American Society for Mechanical Engineers, and a Fellow of the American Institute for Mechanical and Biological Engineering. She has co-authored more than 150 journal articles at the interface of engineering and medicine, she is an editorial board member of eight journals, and a founding member of the Living Heart Project. Ellen received the National Science Foundation Career Award in 2010 for her research on the virtual heart and the Humboldt Research Award in 2016 for her research on the human brain.
CITIUS, ALTIUS, FORTIUS!

What makes HPC actually “high-performing”? Much more than the large-scale computational problems we are facing today and the resulting involvement of state-of-the-art large-scale systems typically mentioned in that context, it is the permanent pursuit of efficiency at all levels to obtain the high performance desired. But what exactly is performance, and how is efficiency defined, given the completely different meanings that exist of both notions? And what is necessary to sustainably ensure that efficiency – including hardware-conscious programming and code tuning, but going far beyond that? Which lessons from HPC related to both algorithm and performance engineering can and should be learnt and adopted also in “normal” programming contexts, outside the high-end systems; and which are the challenges specific to those high-end systems at the eve of exa-scale? Finally, last but not least, how can those contents be taught suitably in an educational context? The talk will address and discuss these questions.

Hans-Joachim Bungartz is a Professor of Informatics and Mathematics at TUM and holds the Scientific Computing chair in TUM’s Informatics Department. After having earned degrees in Mathematics and Informatics from TUM, he became Associate Professor of Mathematics at University of Augsburg, then Full Professor of Informatics at University of Stuttgart, and returned to TUM in 2005. Since 2013, he has been both Dean of Informatics and Graduate Dean, with responsibility of doctoral education TUM-wide. Dr. Bungartz has served on various editorial, advisory, or review boards. In 2011, he became chairman of the DFN. Furthermore, he is a board member of Leibniz Supercomputing Center. In 2016, he joined the steering committee of the Council for Doctoral Education of the European University Association. His research interests are where Scientific Computing, CSE, and HPC meet. This includes parallel computing, hardware-aware numerics, high-dimensional problems, and aspects of HPC software, with applications such as fluid dynamics or plasma physics. Most of his projects are interdisciplinary ones – e.g., he is one of the coordinators of DFG’s Priority Program SPPEXA.
SIMULATION OF COMPLEX SOCIAL PHENOMENA: CONCEPTS AND CHALLENGES

The growing complexity of our world makes it increasingly difficult to understand social phenomena such as migration, social unrest, or consumption patterns, with any reliability. Complex social phenomena differ from natural phenomena in a number of respects: they include agents that have the freedom to choose options using different rationales or no obvious rational at all, they consist of many idiosyncracies that are difficult to include in algorithms and their impacts are spread across diverse areas of public and economic life. Most notably, their impacts transcend both systemic boundaries (between scientific, political, and societal systems, for example) and national boundaries. The lecture will address the complex interdependencies between science and society through the lenses of inter- and transdisciplinary research perspectives. These interdependencies will be examined across a variety of fields, including business, technology, the environment, and society. Within this context, the main task is to identify and characterize common patterns and structures across different social domains.

Dr. Renn is scientific director at the International Institute for Advanced Sustainability Studies (IASS) in Potsdam (Germany) since February, 1, 2016. He continues to serve as acting chair of the Stuttgart Research Center for Interdisciplinary Risk and Innovation Studies at the University of Stuttgart (ZIRIUS) and as scientific director of the non-profit company DIALOGIK, a research institute for the investigation of communication and participation processes. Renn is Adjunct Professor for “Integrated Risk Analysis” at Stavanger University (Norway) and Affiliate Professor for “Risk Governance” at Beijing Normal University.

Ortwin Renn has a doctoral degree in social psychology from the University of Cologne. His career included teaching and research positions at Clark University (Worcester, USA), the Swiss Institute of Technology (Zuerich) and the Center of Technology Assessment (Stuttgart). His honours include the National Cross of Merit Order, an honorary doctorate from the Swiss Institute of Technology, an honorary professorship at the Technical University Munich and the “Distinguished Achievement Award” of the Society for Risk Analysis (SRA)
ON USING SYSTEM DYNAMICS TO BUILD ADAPTIVE CAPACITY WITH SMALL-SCALE FARMERS IN SUB-SAHARAN AFRICA

My keynote lecture discusses a participatory system dynamics project in rural Zambia. I investigate how participatory system dynamics modelling can be adapted to groups at the community level with low formal educational background. I report on a series of interviews and workshops with small-scale farmers in Zambia where we simplified and adjusted the regular model building process and tracked the development of systems thinking competence. Our analyses show that participatory system dynamics is well adaptable to support an audience-specific learning-by-doing approach. The use of pictures, objects and water glasses in combination with the basic aspects of causal loop diagramming makes for a well-balanced toolbox. It provides incentives for engagement through familiar items from participants’ day-to-day practice while at the same time posing conceptual challenges that need to be resolved in the group. The newly acquired understanding is also relevant beyond systems thinking in that it seems to have triggered behavior change in a variety of ways.

Birgit Kopainsky is an associate professor in System Dynamics at the University of Bergen in Norway. She holds a PhD in agricultural economics from ETH Zurich and a master's degree in Geography from the University of Zurich in Switzerland. In her research, she explores the role that system dynamics analysis and modelling techniques play in facilitating transformation processes in social-ecological systems, such as the transition towards sustainable agri-food systems on local, national and international levels. She has done extensive fieldwork in several sub-Saharan African countries and teaches at ETH Zurich as well as at the University of Bergen.
FROM LOCAL MODIFICATIONS TO GLOBAL EFFECTS IN FINITE ELEMENT FLOW SIMULATIONS

We discuss two types of local and computationally inexpensive modifications resulting in finite element approximations of higher accuracy. In case one, we consider a fluid-thermal interaction problem. A local recovery of the discrete flux is performed such that mass conservation on a dual mesh can be guaranteed. The corrected flux enters then into the advective part of the energy equation. To further improve the performance in large scale simulation runs, we use a two-scale time integration scheme in combination with extrapolation techniques and an all-at-once multigrid solver for the flow part. Node-wise defined Uzawa type smoothers guarantee level independent convergence rates for the variable V-cycle. In case two, the flowability in the discrete scheme is locally enhanced such that energy can be preserved. A variational crime analysis then guarantees improved convergence rates in case of non-convex domains with a re-entrant corner. All theoretical results are illustrated by a series of simulations.
OPENSPACE – VISUALIZING THE UNIVERSE

This talk will present and demonstrate the NASA funded open source initiative, OpenSpace, which paves the path for the next generation of public outreach in large scale immersive environments such as dome theaters and planetariums. OpenSpace is also a tool for space and astronomy research as well as a platform for technical visualization research. It opens up the possibilities to dynamically load and visualize data from simulations such as current space weather as well as data from instruments on space crafts. As an example, OpenSpace will, in a live demonstration, be used to show the New Horizons Pluto flyby on July 14th, 2015. A recent feature of OpenSpace is the globe browsing support which enables contextualization of high resolution imagery of planet surfaces. The project builds on a collaboration between Linköping University, The American Museum of Natural History, NASA Goddard Space Flight Center, New York University, University of Utah, and University of Vienna. The remote steering capability of OpenSpace will be demonstrated as the software will be piloted from Norrköping, Sweden.

Professor Anders Ynnerman received a PhD in physics from Gothenburg University, Sweden. During the early 90s, he was at Oxford University, UK, and Vanderbilt University, USA. From 1997 to 2002, he directed the Swedish National Supercomputer Centre, and from 2002 to 2006, he directed the Swedish National Infrastructure for Computing (SNIC). Since 1999, he holds the chair in scientific visualization at Linköping University and is the director of the Norrköping Visualization Center C. Ynnerman is a member of the Swedish Royal Academy of Engineering Sciences and the Royal Academy of Sciences. In 2007, Ynnerman was awarded the Akzo Nobel Science award and the Golden Mouse award for Swedish IT-person of the year. In 2009, he received the Athena Award for best medical clinical research in Sweden and in 2010, he received the Swedish Knowledge Award for dissemination of scientific knowledge to the public. In 2011, he received the IVA gold medal from the King of Sweden and in 2017 he received the King’s medal for his contributions to science.
MESOSCOPIC MODELLING OF ACTIVE MATERIALS: SELFASSEMBLY AND EMERGENT PROPERTIES

Flocks of birds, schools of fishes, nanorobots or bacterial colonies constitute examples of living systems that coordinate their motion, constitute examples of active materials. They are intrinsically out of equilibrium making them very versatile, with a natural tendency to self-assemble. The intrinsic non-equilibrium nature of these materials requires a dynamical approach that consistently captures the different relevant components that determine their behavior. Large system sizes are required to unravel the impact of long-range correlations that characterize them. These correlations lead to dynamical slowing down, hence implying the need for long simulation runs. The computational study of these materials is challenging and benefits from algorithms that show good scalability and can exploit HPC facilities. I will describe the simulation framework adapted to the study of active materials. Such a computational analysis provides insights into the general features determining the emergent properties of this new type of systems.

Director of CECAM, since 2011 he is Full Professor in Condensed Matter Physics at the University of Barcelona. He has developed and exploited mesoscopic computational methods to model the dynamics of soft matter and complex fluids. Recently, he has also extended his interests to study the behavior of biological systems at molecular and cellular scale. He has attracted funding from the Catalan and Spanish Governments, and from the European Union, as well as from industrial companies and private foundations. He has been involved in 54 scientific projects competitively funded, as Principal Investigator. He is member of the External Council Board of the School of Mathematics and Physics of the University of Lincoln (UK). He has published 160 papers in peer reviewed international journals.
DEEP NEURAL NETWORKS IN SIMULATION SCIENCE

During the last few years, the rapid development of deep neural networks has led to remarkable advances in image classification, machine translation, and automatic game playing to name a few. However, for the simulation of complex physical/biological systems these advances remain less utilized. In this presentation we discuss ways in which the remarkable power of deep neural networks in areas of inference and classification can be harvested to address problems that challenge traditional simulation techniques. Through a few concrete examples, we illustrate the potential benefits of a collaborative approach, comprising a combination of classic simulations and deep neural networks, and highlight challenges and open questions associated with such an approach. This work has been done in collaboration with D. Ray (EPFL, CH), S. Ubbliani (USI, CH) and J. Yu (Beihang Uni, China).

After receiving his PhD in 1995 from the Technical University of Denmark, Professor Hesthaven joined Brown University, USA where he became Professor of Applied Mathematics in 2005. In 2013 he joined EPFL as Chair of Computational Mathematics and Simulation Science and since 2017 he serves as Dean of Basic Sciences. His research interests focused on the development, analysis, and application of high-order accurate methods for the solution of complex time-dependent problems, often requiring high-performance computing. Recently he has contributed to the development of reduced basis methods, lately in combination with techniques from machine learning.

He has received several awards for both his research and his teaching, and has published 4 monographs and more than 125 research papers. He is on the editorial board of 8 journals and serves as Editor-in-Chief of SIAM J. Scientific Computing.
SURVIVING THE DATA DELUGE: A SYSTEMS AND CONTROL PERSPECTIVE

The past few years have witnessed a revolution in data collection capabilities: The development of low cost, ultra-low power sensors capable of harvesting energy from the environment has rendered ubiquitous sensing feasible. When coupled with a parallel growth in actuation capabilities, these developments open up the possibility of new technologies that can profoundly impact society, ranging from zero-emissions buildings to “smart” grids and managed aquifers to achieve long term sustainable use of scarce resources. A major road-block to realizing this vision stems from the curse of dimensionality. Successful operation in these scenarios requires the ability to timely extract relevant, actionable information from the very large data streams generated by the ubiquitous sensors. However, existing techniques are ill-equipped to deal with this “data avalanche”.

This talk discusses the central role that systems theory can play in developing computationally tractable, scalable methods for extracting actionable information that is very sparsely encoded in high dimensional data streams. The key insight is the realization that actionable information can be often represented with a small number of invariants associated with an underlying dynamical system. Thus, in this context, the problem of actionable information extraction can be reformulated as identifying these invariants from (high dimensional) noisy data, and thought of as a generalization of sparse signal recovery problems to a dynamical systems framework. While in principle this approach leads to generically nonconvex, hard to solve problems, computationally tractable relaxations (and in some cases exact solutions) can be obtained by exploiting a combination of elements from convex analysis and semi-algebraic geometry. These ideas will be illustrated using examples from several application domains, including autonomous vehicles, computer vision, systems biology and economics. The talk will conclude by exploring the connection between hybrid systems identification, information extraction, and machine learning, and point out to new research directions in systems theory and in machine learning motivated by these problems.
Mario Sznaier is currently the Dennis Picard Chaired Professor at the Electrical and Computer Engineering Department, Northeastern University, Boston. Prior to joining Northeastern University, Dr. Sznaier was a Professor of Electrical Engineering at the Pennsylvania State University and also held visiting positions at the California Institute of Technology. His research interest includes robust identification and control of hybrid systems, robust optimization, and dynamical vision. Dr. Sznaier is currently serving as an associate editor for the journal Automatica and as chair of the IFAC Technical Committee on Robust Control. Past recent service includes Program Chair of the 2017 IEEE Conf. on Decision and Control, General Chair of the 2016 IEEE Multi Systems Conference, Chair of the IEEE Control Systems Society Technical Committee on Computational Aspects of Control Systems Design (2013-2017), Executive Director of the IEEE CSS (2007-2011) and member of the Board of Governors of the CSS (2006-2014). In 2012 he received a distinguished member award from the IEEE Control Systems Society for his contributions to robust control, identification and dynamic vision. A list of publications and current research projects can be found at http://robustsystems.coe.neu.edu
ATOMISTIC MOLECULAR SIMULATIONS FOR PROCESS ENGINEERING: METHODS, TOOLS AND RESULTS

Molecular modeling and simulation has a sound physical basis and is a versatile approach to numerous challenges in chemical engineering and energy technology. It relies on models for the molecular interactions which, once they are parameterized, contain the complete thermodynamic behavior of the considered material. This goes far beyond classical models, such as equations of state which describe e.g. thermal and caloric properties of bulk phases only. Molecular models also contain information on transport properties, the behavior of matter at interfaces, in pores, during phase change processes and under many other conditions. Moreover, the spatial and temporal resolution of simulation is typically many orders of magnitude better than in case of experimental approaches, while similar accuracies can often be reached. The crucial ingredients are molecular models, which nowadays often rely on quantum chemical \textit{ab initio} data, computational tools that embody simulation methods and computing power that is provided by hardware.

Jadran Vrabec is full professor for Thermodynamics and Energy technology at the University of Paderborn, Germany since 2009. His work is centered around molecular modeling and simulation for process and energy engineering applications. After studying process engineering at the Ruhr-University of Bochum, he also accepted his PhD there in 1996. Subsequently to an interim phase working as a management consultant, he became a group leader for molecular thermodynamics at the University of Stuttgart, where he received his habilitation in 2007. Vrabec has co-authored almost 200 peer-reviewed research papers, most of which discuss different aspects of atomistic molecular modeling and simulation methods. He has a strong interest in high-performance computing and the according development of simulation software. Together with his co-authors, he carried out molecular dynamics simulations for the largest system that was described on the atomistic scale. Vrabec is active in different national and European working parties for thermodynamics and molecular simulation.
OPTIMIZATION BY SIMULATION: HEURISTICS AND CERTIFICATES

Many optimization problems in systems and control are NP-hard. One reason of difficulty is the presence of uncertainty because this requires that one deals with many, possibly infinitely many, situations simultaneously. One approach to attack the problem is by simulation: only some instances of the uncertainty are considered and a design which is robust with respect to these cases is performed. But: how good is the design for out-of-sample cases? In other words: how does the quality of the solution extends to new situations? Answering these questions leads to a truly fascinating journey where concepts like risk and complexity find their natural collocation.

Marco Claudio Campi is professor of control and inductive methods at the University of Brescia, Italy. He is the chair of the Technical Committee IFAC on Modeling, Identification and Signal Processing (MISP) and has been in various capacities on the Editorial Board of Automatica, Systems and Control Letters and the European Journal of Control. Marco Campi is a recipient of the "Giorgio Quazza" prize, and, in 2008, he received the IEEE CSS George S. Axelby outstanding paper award for the article "The Scenario Approach to Robust Control Design". He has delivered plenary and semi-plenary addresses at major conferences including SYSID, MTNS, and CDC. Currently he is a distinguished lecturer of the Control Systems Society. Marco Campi is a Fellow of IEEE, a member of IFAC, and a member of SIDRA.
Nigel Davies
Lancaster University | Great Britain

Wednesday, 28 March 2018
11:45 am – 12:30 pm
V 47.03

NEXT GENERATION PHYSICAL ANALYTICS

Weiser’s vision of ubiquitous computing is becoming a reality through technology such as the IoT. A key research challenge lies in providing analytics that capture user interaction with these systems. I will explore this issue using a case study based on pervasive display networks. Traditional signage analytics provide a display-centric view of the world, reporting data on content shown, audience numbers and demographics. This is problematic if we want to understand where, for example, to place content in a network of physically distributed digital signs to optimise content exposure. Synthetic analytics combine mobility simulations with signage analytics data to provide viewer-centric analytics. This approach enables us to ask questions of the analytics from the viewer’s perspective for the first time, transforming the way signage networks, and pervasive IoT systems more generally, can be understood and managed.

Nigel Davies is a Distinguished Professor of Computer Science and Co-Director of the Data Science Institute at Lancaster University. He has held visiting positions at Sony Electronics, Google Research, ETH Zurich, CMU and most recently Università della Svizzera italiana. In addition, Nigel has served as CTO for an SME creating novel IoT systems for the highways sector. His work is in the area of pervasive computing including systems support for new forms of data capture and interaction and is characterized by an experimental approach involving large-scale deployments of novel systems with end-users. Nigel has chaired many of the major conferences in the field, is a former editor of IEEE Pervasive Computing and an Associate Editor of IEEE Transactions on Mobile Computing.
OPTIMIZATION UNDER UNCERTAINTY FOR COMPLEX PDE MODELS IN HIGH DIMENSIONS

We consider optimization problems governed by PDEs with infinite dimensional random parameters. Such problems arise in multiple settings, including optimal design/control of uncertain systems, inverse problems governed by uncertain forward problems, and Bayesian optimal experimental design. The uncertainty in the PDEs leads to an uncertain objective function and hence a PDE-constrained stochastic optimization problem. Conventional Monte Carlo approximation of the objective results in a deterministic optimization problem with as many PDE constraints as there are sample points, which is prohibitive to solve. We present high-order derivative-based approximations of the parameter-to-objective maps that, in combination with randomized algorithms and used as control variates, exploits the structure of the maps (smoothness, low effective dimensionality) and leads to several orders of magnitude acceleration of Monte Carlo for a turbulent flow control problem with $O(10^6)$ uncertain parameters.

Dr. Omar Ghattas is a Professor of Geological Sciences and Mechanical Engineering at the University of Texas at Austin. He is also the Director of the Center for Computational Geosciences and Optimization in the Institute for Computational Engineering and Sciences (ICES) and holds the John A. and Katherine G. Jackson Chair in Computational Geosciences. He is also a member of the faculty in the Computational Science, Engineering, and Mathematics (CSEM) interdisciplinary PhD program in ICES, and holds courtesy appointments in Computer Science and Biomedical Engineering. He has general research interest in forward and inverse modeling, optimization, and uncertainty quantification of large-scale complex mechanical, geological, and biological systems. He received the ACM Gordon Bell Prize in 2003 (for Special Achievement) and again in 2015 (for Scalability), and was a finalist for the 2008, 2010, and 2012 Bell Prizes. He is a Fellow of the Society for Industrial and Applied Mathematics (SIAM).
DATA-DRIVEN COMPUTING

We develop a new computing paradigm, which we refer to as Data-Driven Computing, according to which calculations are carried out directly from experimental material data and pertinent kinematic constraints and conservation laws, such as compatibility and equilibrium, thus bypassing the empirical material modeling step of conventional computing altogether. Data-driven solvers seek to assign to each material point the state from a prespecified data set that is closest to satisfying the conservation laws. Equivalently, data-driven solvers aim to find the state satisfying the conservation laws that is closest to the data set. The resulting Data-driven problem thus consists of the minimization of a distance function to the data set in phase space subject to constraints introduced by the conservation laws. We demonstrate the Data-driven paradigm and investigate the performance of Data-driven solvers by means of several examples of application, including statics and dynamics of nonlinear three-dimensional trusses, and linear and nonlinear elasticity. In these tests, the Data-driven solvers exhibit good convergence properties both with respect to the number of data points and with regard to local data assignment, including noisy material data sets containing outliers. The variational structure of the Data-driven problem also renders it amenable to analysis. We find that the classical solutions are recovered in the case of linear elasticity. We identify conditions for convergence of Data-Driven solutions corresponding to sequences of approximating material data sets. Specialization to constant material data set sequences in turn establishes an appropriate notion of relaxation. We find that relaxation within the Data-Driven framework is fundamentally different from the classical relaxation of energy functions. For instance, we show that in the Data-Driven framework the relaxation of a bistable material leads to effective material data sets that are not graphs. I will finish my presentation with highlights on work in progress, including closed-loop Data-Driven analysis and experiments, Data-Driven molecular dynamics, Data-Driven inelasticity and publicly-editable material data repositories and data management from a Data-Driven perspective.
Professor Michael Ortiz received a BS degree in Civil Engineering from the Polytechnic University of Madrid, Spain, and MS and PhD degrees in Civil Engineering from the University of California at Berkeley.

From 1984-1995 he held a faculty position in the Division of Engineering of Brown University, where he carried out research activities in the fields of mechanics of materials and computational solid mechanics. He is currently the Dotty and Dick Hayman Professor of Aeronautics and Mechanical Engineering at the California Institute of Technology, where he has been in the faculty since 1995.

Professor Ortiz is or has been a Fulbright Scholar, a Sherman Fairchild Distinguished Scholar at Caltech, Midwest and Southwest Mechanics Seminar Series Distinguished Speaker, a Fellow and an elected member-at large of the US Association for Computational Mechanics, Hans Fischer Senior Fellow of the Institute of Advanced Studies of the Technical University of Munich, an elected Fellow of the American Academy of Arts & Sciences and an elected member of the US National Academy of Engineering.

Furthermore, he is the recipient of the Alexander von Humboldt Research Award for Senior US Scientists, the IACM International Computational Mechanics Awards for Research, the USACM Computational Structural Mechanics Award, the ISI Highly Cited Researcher Award, the inaugural 2008 Rodney Hill Prize conferred every four years by the IUTAM and the Timoshenko Medal of the American Association of Mechanical Engineers.

He has served in the University of California Office of the President Science and Technology Panel and in the Lawrence Livermore National Laboratory Predictive Science Panel. He has been editor of the Journal of Engineering Mechanics of ASCE and of the Journal of Applied Mechanics of the ASME, associate editor of the journal Modeling and Simulation in Materials Science and Engineering and of the Journal for Computational Mechanics, and is presently associate editor of the Journal for the Mechanics and Physics of Solids and of the Archive for Rational Mechanics and Analysis.

Actually, he holds an h-index of 78 at Thomson Reuter’s ISI Web of knowledge.
Mini Symposia & Postertracks
## Mini Symposium 1: Material Design: Multi-scale and Multi-field Simulations of Materials

Chair: JP Keip

Room: 47.05

### Postertrack

- Miguel Bessa
- Anne Romer
- Tobias Holicki
- Andreas Hofmann
- Philip Tempel
- Andreas Schmidt

### Postertrack

- Jan Hasenauer
- Nicole Radde
- Syn Schmitt
- Tim Ricken
- Guang Yang

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## Mini Symposium 3: Dynamical Systems: Reduction, Optimization and Control

Chair: Prof. Allgöwer

Room: 9.01

### Postertrack

- Prof. Radde, Prof. Röhrle, Prof. Ehlers

### Postertrack

- Isabelle Faillie
- Roland Masson
- Unice
- Michael Dumbser
- Martin Schneider

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## Mini Symposium 4: Coupled Problems in Biomechanics and Systems Biology

Chair: Prof. Radde, Prof. Röhrle, Prof. Ehlers

Room: 47.03

### Postertrack

- Prof. Helmig

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## Mini Symposium 5: Multi-phase and Multi-physics Modelling

Chair: Prof. Helmig

Room: 7.01

### Postertrack

- Miguel Bessa
- Anne Romer
- Tobias Holicki
- Andreas Hofmann
- Philip Tempel
- Andreas Schmidt

### Postertrack

- Jan Hasenauer
- Nicole Radde
- Syn Schmitt
- Tim Ricken
- Guang Yang

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# Day 2: 26 March 2018

**2:00 pm – 3:30 pm**

- **Mini Symposium 1:** Material Design: Multi-scale and Multi-field Simulations of Materials
- **Mini Symposium 2:** Dynamical Systems: Reduction, Optimization and Control
- **Mini Symposium 3:** Coupled Problems in Biomechanics and Systems Biology
- **Mini Symposium 4:** Multi-phase and Multi-physics Modelling

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<td>Prof. Helmig</td>
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MATERIAL DESIGN: MULTI-SCALE AND MULTI-FIELD SIMULATIONS OF MATERIALS

DATA-DRIVEN DESIGN OF MULTI-SCALE MATERIALS AND STRUCTURES

Miguel Bessa, Delft University of Technology

Data-driven research has the potential for groundbreaking achievements in the design of materials and large-scale engineering structures. However, these approaches to design are limited by the substantial computational expense of building large databases, especially when modeling irreversible processes such as plasticity and damage. A new computational framework integrating the recently developed self-consistent clustering analysis method is shown to address this longstanding challenge, opening avenues to the discovery of innovative materials with new capabilities in an era of high-throughput computing (“big-data”).

Postertrack contributions:
Tobias Willerding (PP1.002); Jim Magiera (PP1.003); Lukas Ostrowski (PP1.007); Daniel Vallicotti (PP1.008); Sami Bidier (PP1.009); Philipp Rehner (PP1.010); Matthias Rambausek (PP1.011); David Kreplin (PP1.012); Marco Salvalaglio (PP1.013); Dennis Rapp (PP1.015); Anand Krishnamoorthy (PP1.016).
DYNAMICAL SYSTEMS: REDUCTION, OPTIMIZATION AND CONTROL

DATA-DRIVEN INFERENCE OF CONTROL THEORETIC SYSTEM PROPERTIES

Anne Romer, University of Stuttgart

Since the amount of available data is increasing rapidly, there has been an increasing interest in what is called data-driven control. One complementary approach to the direct controller design from data is to learn and analyze certain system properties from data first, since they allow for the direct application of well-known feedback theorems for controller design. Hence, by learning such properties from data, we obtain insights to the a priori unknown system, we are not bound to a certain controller structure beforehand while still providing control theoretic guarantees for the closed-loop behavior. Along those lines, we present sampling strategies to iteratively determine the operator gain, the shortage of passivity and conicity of linear time-invariant systems, whose input-output map remains undisclosed. These sampling strategies are based on gradient dynamical systems and saddle point flows, which asymptotically reveal the true system properties.

ANALYSIS OF NETWORKED SYSTEMS OVER SWITCHING TOPOLOGIES

Tobias Holicki, University of Stuttgart

Novel criteria for robust stability and performance analysis are proposed for a class of networked systems with a switching communication structure. In contrast to other approaches, our results are based on recent separation techniques from robust control. These offer substantial extra flexibility and pave the way for covering more general interconnection structures that are affected by heterogeneous uncertainties. The benefits of the proposed approach are illustrated by means of several numerical examples. Moreover, we address the potentials to merge these analysis techniques with distributed controller synthesis algorithms that we recently developed for fixed interconnection structures.

UNCERTAINTY IN CONTROLLED MULTIBODY SYSTEMS

Andreas Hofmann, University of Stuttgart

Model-based controller design for multibody systems implies exact knowledge of the system dynamics, and the success and the performance are related to the accuracy of the underlying system model. Consequently, a systematically misbehaving controller may arise if model uncertainties are not considered in the design process. In this presentation new methods and ideas for designing model-based robust controllers for multibody systems based on fuzzy arithmetical uncertainty modeling are presented. Fuzzy sets provide a mathematical formulation for possibilisty theory and possibilistic uncertainty models, so that fuzzy arithmetical concepts are well suited for the uncertainty modeling and analysis. Moreover, the presented method allows to incorporate a maximum of available data and knowledge about the shape of the inherent uncertainty into the resulting controller design.
IMPROVED MODELING OF KINEMATICS AND DYNAMICS OF CABLES FOR USE IN CABLE-DRIVEN PARALLEL ROBOTS

Philipp Tempel, University of Stuttgart

Cable-driven parallel robots make use of elastic cables for force and motion transmission from the driving winches to the mobile platform. The system is inherently susceptible to transversal cable vibration stemming from jerky motion of the platform as well as cable winding and guiding. To improve precision and stiffness of cable robots, the cable motion must explicitly be considered in simulation and control. In this poster, we present different approaches to modeling the cable shape based on the static model first derived by Irvine. Two main approaches are presented, one based on discretization of the cable into segments yielding high dimensional systems, the other being based on Rayleigh-Ritz modal superposition yielding lower dimensional systems. Additionally, the static and dynamic cable force transmission is evaluated against existing models such as four-element or Flory models. Furthermore, overall model validity and applicability to improving accuracy and stiffness is shown.

FEEDBACK CONTROL OF PARAMETRIZED PDES VIA MODEL ORDER REDUCTION AND DYNAMIC PROGRAMMING PRINCIPLE

Andreas Schmidt, University of Stuttgart

We investigate infinite horizon optimal control problems for nonlinear parametrized partial differential equations via the famous dynamic programming principle of Bellman by solving Hamilton-Jacobi-Bellman (HJB) equations. Classical discretization techniques for HJB equations are prone to the so-called curse of dimensionality, rendering these methods infeasible already in low-dimensional spaces (say 5–8 dimensions). By combining recent model order reduction techniques for feedback control problems and enhancements like parameter partitioning with efficient approximation schemes for HJB equations, we arrive at reduced problems that can be solved efficiently. Our approach is divided in an offline and online phase, where the online phase is substantially sped up by precalculations that have to performed once in an offline step. Numerical examples for linear and nonlinear flow problems illustrate the effectiveness of the proposed method.

Postertrack contributions:

Christian Kleinbach & Jörg Fehr & Oleksandr Martynenko & Syn Schmitt (PP3.045); Dennis Grunert & Kevin Carlberg & Jörg Fehr (PP3.046); Abelardo Rodriguez Pretelin & Wolfgang Nowak (PP3.047); Steffen Linsenmayer & Frank Allgöwer (PP3.048); Ehsan Sharafian Ardakani & Henrik Ebel & Peter Eberhard (PP3.049); Dominik Hamann & Peter Eberhard (PP3.050); Mylena Mordhorst (PP3.051); Johannes Köhler (PP3.052); Fatemeh Ansarieshlaghi & Peter Eberhard (PP3.053); Christian A. Rösinger (PP3.054); Jannik Haas & Wolfgang Nowak (PP3.055); Nehzat Emamy & Pascal Litty & Miriam Mehl (PP3.056); Sergey Oladyshkin & Anneli Guthke & Farid Mohammadi & Rebekka Kopmann & Wolfgang Nowak (PP3.057); Matthias Lorenzen & Frank Allgöwer (PP3.058); Sebastian Most & Wolfgang Nowak & Marco Dentz & Branko Bijeljic & Diogo Bolster (PP3.059); Bastian Hilder (PP3.060); Malte Heckelen (PP3.061); Roman Föll (PP3.062).
COUPLED PROBLEMS IN BIOMECHANICS AND SYSTEMS BIOLOGY

ON THE PARAMETERISATION OF MULTI-SCALE MODELS IN LIFE SCIENCES

Jan Hasenauer, Helmholtz Center Munich

Mechanistic computational models are powerful tools in modern life sciences. Similar to experimental techniques, mechanistic models facilitate an assessment of hypothesis testing. To achieve this, the unknown model parameters have to be estimated from experimental data. For stochastic processes on multiple time and length scales, parameter estimation is often still intractable. Here, we present established Approximate Bayesian Computation (ABC) - Sequential Monte Carlo (SMC) methods which are conceptually applicable for the calibration of stochastic multi-scale models but computationally demanding. To facilitate the application of these methods to computationally intensive models, we introduce pyABC, an open-source Python toolbox with high-performance computing (HPC) capabilities which offers several features enhancing computational efficiency. We demonstrate pyABC using multi-scale models for tumor growth and immune response. For both applications, pyABC achieves better results than manual tuning and enables an assessment of parameter and prediction uncertainties.

INFEERENCE OF FINITE MICTURE MODELS WITH BINNED SINGLE CELL DATA

Nicole Radde, University of Stuttgart

Finite mixture models have successfully been used to analyze a variety of biological data. Recent examples include single cell data and the quantification of cell-to-cell heterogeneity or the classification of cancer subtypes. Calibration of these models to experimental data is challenging for uncensored data and also for binned data, as often available in practice. Here we investigate the problem of parameter estimation and model selection for finite mixture models from a theoretical perspective and on a real case study with time lapse microscopy data. In statistics it has long been known that the calibration of mixture models constitutes an ill-posed problem. We illustrate this fact on mixtures of different distribution families and discuss the effect of binning on this inverse problem. We demonstrate that a proper treatment of binning can in fact facilitate estimation of the number of mixtures compared to inference from uncensored data, an at first glance surprising result.

METHODS AND MODELS TO STUDY BIOMECHANICS AND MOTOR CONTROL

Syn Schmitt, University of Stuttgart

The dynamics of a biological system is truly unique. No other system, even highly sophisticated, engineered structures do not show the same inherent complexity neither in their structure nor in their functioning. To understand biological systems better, models could come into play. In this talk, methods and models are presented to study biological locomotion. Spanning multiple spatial and temporal scales, being developed over a long time of evolution, and having data-poor and datarich regimes available for validation, modelling a biological system proves a demanding challenge. However, being able to simulate a biological motion using neuro-musculo-skeletal models opens up the space to answer questions like, as to whether non-linearities in biology are a work around due to available building materials or a design feature to enable simpler motion planning and execution?
UNCERTAINTY QUANTIFICATION OF MULTI-X LIVER LOBULE DAMAGE SIMULATION

Tim Ricken, University of Stuttgart

The human liver regulates metabolism in a complex time depending and non-linear coupled function-perfusion mechanism. The viability of the organ is affected by a failure in the liver structure, e.g. lipid accumulation. We present a computational multi-X model for the human liver which is composed of three coupled submodels for the organ, lobule- and cell-scale. Thus, the effect of inhomogenously distributed growing fat vacuoles in the liver cells could be computed. To address uncertainty quantification, two promising approaches of analytical and stochastic sensitivity analysis will enhance the deterministic structural analysis. The variational sensitivity analysis is used to capture the impact of different parameters as continuous functions. An advantage is the accurate approximation of the solution space and the efficient computation time. In the probabilistic sensitivity analysis, we use Bayes statistics will enable to receive accurate information with just a few simulations.

Postertrack contributions:

Karsten Kuritz (PP4.063); Ewa Anna Oprzeska-Zingrebe (PP4.064); Jonas Landgesell & Christian Holm & Patrick Kreissl & Georg Rempfer & Florian Weik & Kai Szutter (PP4.065); Wolfgang Halter (PP4.066); Stefan Engblom (PP4.067); Simon Wolfen (PP.068); Ekin Altan & Leonardo Gizzi & Sergey Oladyshkin & Oliver Röhrle (PP4.069); Tobias Koeppi & Paolo Zunino & Barbara Wohlmuth & Ettore Vidotto (PP4.071); Daniela Stöhr (PP4.072); Dirk Imig (PP4.073); Frank Maier (PP4.074); Davina Fink (PP4.075); Sergio Morales & Oliver Röhrle (PP4.076); Patrick Schröder & Arndt Wagner & Daniela Stöhr & Rehm Markus & Wolfgang Ehlers (PP4.077); Debdas Paul & Nicole Radde; Sergio Morales & Oliver Röhrle (PP4.079); Maria Hammer & Michael Günther & Daniel F. B. Haefelfe & Johannes Walter & Syn Schmitt (PP4.080); Antje Jensch & Katharina Bitschar & Nicole Radde & Monilola Olayioye (PP4.081); Nehzat Emamy & Thomas Ertl & Dominik Göddeke & Thomas Kotlin & Aaron Krämer & Michael Krone & Benjamin Maier & Miriam Mehl & Tobias Rau & Oliver Röhrle (PP4.082); Christian Bleiler (PP4.083); Klaudius Scheufele & Andreas Mang (PP4.084); Katrin Stollenmaier (PP4.085).
MULTI-PHASE AND MULTY-PHYSICS MODELLING

HYBRID FINITE VOLUME SCHEMES FOR SEDIMENTARY BASIN SIMULATION IN COMPLEX SETTINGS

Isabelle Faille, IFP Energies nouvelle

Basin simulation aims at reconstructing the evolution through geological time of the porous sedimentary layers and the fluid that fill in. In complex tectonic settings, it needs to account for faults that become a major element of basin evolution. At basin scale, faults are mainly slip surfaces but also zones of deformed rocks that can have a major impact on fluid flow pathways. We present a modeling approach in which a basin is represented by an evolving unstructured mesh that follows sedimentary layers’ deformation. Faults are handled as pairs of internal boundaries across which the mesh is non-matching and that can therefore slide one past the other. Mass and heat transfer are computed using the Hybrid Finite Volume Scheme able to handle properly the deformed and non matching grids. We illustrate how this scheme can be associated to a double layer interface fault model to simulate fluid flow within the fault zone and account for the different fault behaviors.

A DOMAIN DECOMPOSITION METHOD TO COUPLE NONISOTHERMAL COMPOSITIONAL GAS LIQUID DARCY AND FREE GAS FLOWS

Roland Masson Unice, Université de Nice Sophia-Antipolis

A domain decomposition algorithm is introduced to couple nonisothermal compositional gas liquid Darcy and free gas flow and transport. At each time step, our algorithm solves iteratively the nonlinear system coupling the nonisothermal compositional Darcy flow in the porous medium, the RANS gas flow in the free-flow domain, and the transport of the species and of energy in the free-flow domain. In order to speed up the convergence of the algorithm, the transmission conditions at the interface are replaced by Robin type boundary conditions. The Robin coefficients are obtained from a diagonal approximation of the Dirichlet to Neumann operator related to a simplified model in the neighbouring subdomain. The efficiency of our domain decomposition algorithm is assessed on several test cases focusing on the modeling of the mass and energy exchanges at the interface between the geological formation and the ventilation galleries of geological radioactive waste disposal.

HIGH ORDER ADER SCHEMES FOR A SYMMETRIC HYPERBOLIC MODEL OF COMPRESSIBLE TWO-PHASE FLOWS

Michael Dumbser, University of Stuttgart

In this talk we present preliminary results obtained with high order ADER discontinuous Galerkin and finite volume schemes for a new class of symmetric hyperbolic models for compressible two-phase flows recently developed by E. Romenski. The governing PDE are a multi-material extension of the unified Godunov-Peshkov-Romenski model of continuum mechanics that is able to describe fluid mechanics and solid mechanics within one single set of governing equations. We show results for one-dimensional test problems in order to validate the mathematical model and the employed numerical techniques.

References


NONLINEAR FINITE-VOLUME SCHEMES FOR COMPLEX FLOW PROCESSES AND CHALLENGING GRIDS

Martin Schneider, University of Stuttgart

The numerical simulation of subsurface processes requires efficient and robust methods due to the large scales and the complex geometries involved. To resolve such complex geometries, corner-point grids are the industry standard to spatially discretize geological formations. Such grids include non-planar, non-matching and degenerated faces. The standard scheme used in industrial codes is the cell-centered finite-volume scheme with two-point flux (TPFA) approximation, an efficient scheme that produces unconditionally monotone solutions. However, large errors in face fluxes are introduced on unstructured grids. The authors present a nonlinear finite-volume scheme applicable to corner-point grids, which maintains the monotonicity property, but has superior qualities with respect to face-flux accuracy. The scheme is compared to linear ones for complex flow simulations in realistic geological formations.

A HYBRID DSMC/NAVIER-STOKES FRAMEWORK TO SOLVE THE COUPLED CHANNEL FLOW AND RAREFIELD POROUS MEDIA FLOW

Guang Yang, University of Stuttgart

Coupled channel and porous media flow has been a topic of extensive interest for decades. However, the current models and theories are mainly applicable for low speed, incompressible, and continuum flows. In many emerging technologies, for example, transpiration cooling, the gas flow in the porous media can be rarefied, as the length scale of the pore size may be down to micro- or nanometer. For fluid flow in the transition and free molecular regimes (Kn > 0.1), the continuum hypothesis is no longer applicable. However, the flow in the bulk of the channel is still in the continuum regime, which can be described by the Navier-Stokes equations. In the present study, a hybrid DSMC/Navier-Stokes computational framework is developed in OpenFOAM to solve the coupled system. A direct simulation Monte Carlo (DSMC) method is used for the rarefied porous media flow and the Navier Stokes equations for compressible flow are solved for the channel flow. The momentum and heat transport characteristics at the interface are investigated in detail. The accuracy and efficiency of the present method have also been evaluated.

Postertrack contributions:

Jan Giesselmann (PP5.086); Markus Köppel (PP5.088); Corrado Sotgiu (PP5.100); Alexander Straub (PP5.107); Lukas Eurich & Shahla Shahmoradi & Arndt Wagner & Wolfgang Ehlers (PP5.108); Birane Kane (PP5.114); Julian Valentin (PP5.117); Dominik Wittwar (PP5.120); Serena Vangelatos & Claus-Dieter Munz (PP5.121); David Seus (PP5.124).
### Tuesday, 27 March 2018
**11 am – 12:30 pm**

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<th>Mini Symposium 2</th>
<th>Mini Symposium 6</th>
<th>Mini Symposium 7</th>
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<tr>
<td><strong>Title</strong></td>
<td>High Performance Simulations across Computer Architectures</td>
<td>Cyber Infrastructure and Beyond</td>
<td>Reflexion and Contextualisation</td>
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<td><strong>Chair</strong></td>
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<td><strong>Room</strong></td>
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<td><strong>Tristan Bereau</strong></td>
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<td><strong>Peter Reimann</strong></td>
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<td><strong>Philipp Marquetand</strong></td>
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<td><strong>Michael Lahner</strong></td>
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HIGH PERFORMANCE SIMULATIONS ACROSS COMPUTER ARCHITECTURES

INTERMOLECULAR POTENTIALS FROM MACHINE LEARNING ACROSS CHEMICAL SPACE

Tristan Bereau, Max Planck Institute for Polymer Research

Classical intermolecular potentials typically require an extensive parametrization procedure for any new compound considered. To do away with prior parametrization, I will describe a combination of physics-based potentials with machine learning that is transferable across small neutral organic molecules made of H, C, N, and O atoms. Unlike other potentials, the model is transferable in its ability to handle new molecules and conformations without explicit prior parametrization. I will describe applications on gas-phase dimers and discuss perspectives toward the condensed phase.

MACHINE LEARNING POTENTIALS FOR MOLECULAR DYNAMICS

Philipp Marquetand, University of Vienna

Machine learning is used to find the relationship between the nuclear geometry of a molecule and the corresponding properties, like the potential energy or the dipole moment. In this way, the machine learning algorithm – an artificial neural network in this case – serves as a highly accurate and extremely fast tool during the simulation of molecular dynamics, i.e., the motion and behavior of a molecule in time. Different developments will be presented, e.g., how the neural networks learn to assemble small, known molecules serving as building blocks to predict the properties of a large unknown molecule. As an application, calculations of infrared spectra obtained via molecular dynamics simulations will be shown.

MINIMALLY INVASIVE INTEGRATION OF TREE-STRUCTURED CARTESIAN GRIDS IN EXISTING APPLICATIONS

Michael Lahnert, University of Stuttgart

We present our approach for minimally invasive integration of dynamically-adaptive tree-structured grids at the example of the molecular dynamics (MD) simulation code ESPResSo. It includes an implementation of the Lattice-Boltzmann method (LBM) to subject a molecular ensemble to a background flow as well as a continuous representation of the electrokinetic equations. We port the grids of ESPResSo’s physical subsystems to an extended version of p4est, a well-known and scalable library for tree-structured Cartesian grids. Our contribution to p4est allows simpler integration into existing applications. As not all grids are discretized in the same way, we use independent p4est instances for each algorithm and describe our approach for reducing communication in the coupling scheme. We show results and scalability tests for the individual components as well as for the integrated application on different hardware architectures.
INTERPOLATION OF POTENTIAL ENERGY SURFACES USING GAUSSIAN PROCESS REGRESSION

Alexander Denzel, University of Stuttgart

In this work we are combining methods of quantum mechanics with machine learning methods to find interesting geometries of molecules and other useful properties of chemical systems. One of the fundamental problems in theoretical chemistry is the steep scaling of the calculations that are necessary to determine the energy and its derivatives in a chemical system. We use machine learning methods like neural networks and Gaussian process regression (GPR) to interpolate between obtained energies. GPR is easy and fast to set up for a new system. Furthermore, formulated in a Bayesian setting, it has the capability of giving uncertainty measurements and the possibility of optimizing its parameters with e.g. the maximum likelihood method. We apply this method to interpolate several energy surfaces to do geometry optimization and reaction rate calculations that incorporate quantum mechanical tunneling with fewer electronic structure calculations and therefore, faster than before.
CYBER INFRASTRUCTURE AND BEYOND

DATA PROVISIONING IN SIMULATION WORKFLOWS

Peter Reimann, University of Stuttgart

The input data of computer-based simulations often come from diverse data sources that manage data in a multiplicity of proprietary formats. Corresponding simulation workflows thus have to carry out many complex data provisioning tasks. These tasks filter and transform heterogeneous input data in such a way that underlying calculation tools are able to ingest them. So, scientists have to spend much effort to implement many low-level data transformations. This talk covers a novel pattern-based approach that conquers the data complexity associated with simulation workflows and that completely removes the burden from scientists to implement low-level data transformations. Instead of designing many workflow tasks, scientists only need to select a small number of abstract patterns to describe a high-level simulation process. Furthermore, scientists are familiar with the parameters to be specified for the patterns, because these parameters are related to their domain-specific methodology.

TRANSPARENT DATA EXCHANGE IN SIMULATION CHOREOGRAPHIES

Michael Hahn, University of Stuttgart

Data provisioning, management and transformation are crucial tasks in scientific simulations, especially if multiple simulations are coupled as so-called multi-* simulations. The notion of choreographies will enable scientists to model such coupled simulations from a global perspective through the interconnection of different scientific workflows and simulation software without the need to directly provide complex technical details. To reflect data-related aspects on the level of such simulation choreographies, we introduced the notion of data-aware choreographies through our concepts for transparent data exchange (TraDE). Our main goals are to ease the modeling of coupled simulations and their data; provide continuous, uniform access to simulation data; automate and hide data management, exchange and transformation tasks from scientists wherever possible; and provide an integrated end-to-end tool support for the modeling and execution of data-aware choreographies.

UTILIZING NETWORKED MOBILE DEVICES FOR SCIENTIFIC SIMULATIONS

Christoph Dibak, University of Stuttgart

Emerging augmented reality devices enable novel, interactive simulations. Simulation results no longer need to be viewed on a computer screen but can be overlayed over real-world objects like complex machinery. This supports engineers in making better decisions in the field. However, having interactive simulation results available on mobile devices like augmented reality headsets is challenging since such battery-powered mobile devices are restricted in computational power, have limited energy resources, and are subjected to intermittent connectivity. Additionally, the execution of simulations is hard to distribute between heterogeneous devices. In our research, we developed different methods that can be used for the distribution of the computation between mobile device and remote server. Our approaches significantly improve latency, dynamically adapt quality, and provide simulation results even in harsh environments.
"WORLD CLIMATE": CAN ROLE-PLAY WITH INTERACTIVE SIMULATIONS ENHANCE CLIMATE CHANGE KNOWLEDGE, AFFECT AND INTENT TO ACT?

Juliette Rooney-Varga (University of Massachusetts, Lowell), John Sterman (MIT Sloan School of Management), Eduardo Fracassi (Instituto Tecnologico de Buenos Aires), Travis Franck (Climate Interactive), Florian Kapmeier (Reutlingen University, ESB Business School), Victoria Kurker (University of Massachusetts, Lowell), Ellie Johnston (Climate Interactive), Andrew Jones (Climate Interactive), Kenneth Rath (Sagefox Consulting)

There is an urgent need for communication tools that offer scientifically rigorous information while motivating informed action on climate change. Conventional communication approaches have largely failed to close the gap between scientific and public understanding of the threats posed by climate inaction. Indeed, research shows that showing people research is not effective. Here, we describe the impact of a new approach to climate communication: a simulation-based roleplay that combines a social, engaging role-play of climate decision-making with an interactive computer model that provides immediate feedback on the expected outcomes of those decisions. In particular, we analyze the impact of the World Climate simulation, in which participants take on the roles of delegates to the UN climate negotiations and are challenged to create an agreement that meets international goals. Their decisions are entered into the peer-reviewed interactive computer model C-ROADS (Climate Rapid Overview and Decision Support) that provides immediate feedback about the resulting climate impacts. Thus, participants explore the climate system through the C-ROADS model while experiencing the social dynamics of decision-making through role-play. Results showed significant gains in climate change knowledge, affect, intent to take action, and desire to learn. Results show feedback between gains in affective engagement, particularly feelings of urgency, and gains in knowledge about climate change. Gains in urgency, but not knowledge, were associated with gains in intent to act and desire to learn more. Gains were just as strong among participants who oppose government regulation, suggesting the simulation’s potential to reach across political divides. These findings show that simulations like World Climate offer a climate change communication tool that enables people to learn and feel for themselves, which together have the potential to motivate action informed by science.

Postertrack contributions:

Tom Poljansek (PP7.129), Maximilian Happach & Meike Tilebein (PP7.130).
Poster Session
At the SimTech 2018 conference, about 130 young researchers take the opportunity to present their recent work during the poster session. Next to the official poster session on Tuesday, 27 March 2018, from 2:00 pm to 3:30 pm, all posters can be visited during the whole conference on the ground and lower floor of the building Pfaffenwaldring 47. Where you can find the different topics can be seen in the plans below.

At the end of the conference, on Wednesday, 28 March 2018, at 3:30 pm, the Best Poster Award sponsored by the Industrial Consortium SimTech e. V. will be awarded.
Pfaffenwaldring 47
Lower Floor
**PP1.000**

<table>
<thead>
<tr>
<th><strong>A Variational Framework for Distance-Minimizing Data-Driven Computing Method</strong></th>
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<td><strong>Lu Trong Khiem Nguyen, Matthias Rambausek, Mark-André Keip</strong></td>
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The distance-minimizing data-driven computing method initiated by Kirchoerfer and Ortiz [1] is revisited in the present work. Basically, a boundary value problem of continuum mechanics consists of three ingredients: The compatibility condition on the primary field, the conservation laws, and the material laws that relate the work conjugates such as the linearized strain and the Cauchy stress. The material laws are usually expressed in terms of a functional relationship that fits empirical observations based on experimental data. Thus, there are uncertainties in this approach of calibrating the constitutive laws. In the data-driven computation such functional relation is replaced with an abundant collection of material data. In this manner, we may control the errors in the material laws, conservations laws and compatibility conditions in contrast to the classical approach in which one may produce high numerical precision using FEM with material laws of far less accuracy. The data-driven problem can be expressed as an optimization problem: Find the point in the collection of material data points that minimizes the errors in the conservation laws, compatibility conditions and essential constraints [1,2]. The present contribution proposes a variational framework for the distance-minimizing method using Lagrange multipliers for both the conservation laws and the compatibility condition in the continuous setting [3]. An interpretation of the resulting algorithm as a staggered scheme is also provided. As a consequence, the Galerkin-based methods with different possibilities of interpolation functions can be used. Several representative examples are illustrated in order to justify the proposed variational formulation.


**PP1.001**

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<tr>
<th><strong>Two-Scale Reduced Basis Homogenization under Large Deformations</strong></th>
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<td><strong>Oliver Kunc, Felix Fritzen</strong></td>
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A new solution method for the mechanical homogenization problem for hyperelasticity under large deformations is presented. We develop a reduced basis (RB) homogenization technique in the spirit of [Fritzen, Leuschner; CMAME 2013] and [Fritzen, Kunc; submitted 2017] but for solids undergoing infinite deformations. The main novelties consist of

- comparison of different reduced bases for kinematic quantities
- a posterior error indication (online).

Assuming the paradigm of scale-separability, the starting point is a reduced order model with a RB for the fluctuations of the microscopic deformation gradient. In order to increase the already significant speed-ups and in order to improve on the robustness, alternative parameterizations of local kinematic
fields like the deformation gradient are investigated. The RB-induced error is discussed. Prospects of a generalization to dissipative materials are given.

<table>
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<tr>
<th>PP1.002</th>
<th>Multiscale simulation of phase change</th>
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<td>Tobias Willerding, Manfred Bischoff</td>
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Iron is an interesting material as it has two different lattice structures, body-centered cubic (bcc) and face-centered cubic (fcc). The transition between these two lattice structures can be modeled with molecular dynamics (MD). However, in recent years, multiscale simulation, the coupling of different theories with different length and time scales has become popular. A method to couple finite elements and molecular dynamics is presented, which can also handle transition from one lattice structure to another. In order to achieve this, one possible way is to implement molecular dynamics as a "material model" of the finite element level, with one MD sub problem with periodic boundary conditions at each Gauss point. Another possible solution is to develop a bridging interface that can handle lattice transition. Approaches to both ideas will be presented.

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<tr>
<th>PP1.003</th>
<th>A Hybrid Particle-Continuum Multiscale Two-Phase Flow Model</th>
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<td>Jim Magiera</td>
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We consider a sharp interface approach for compressible liquid-vapor interaction, and in particular the description of liquid droplet dynamics with phase change. At the phase interface a Riemann problem has to be solved for which additional coupling conditions (i.e. kinetic relations) are needed. However, in most cases the physically correct choice remains unclear. In our contribution we present a multiscale Riemann-solver that is based on microscopic molecular dynamics simulations and bypasses the formulation of additional closure relations. Instead of performing the microscale simulations every single time, we apply a dynamic machine learning approach to train a surrogate model in order to reduce the computational effort.

<table>
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<tr>
<th>PP1.004</th>
<th>Substituting FE analysis of cyclic processes by a space-time reduced order model</th>
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<td>Mohammad Reza Hassani, Felix Fritzen</td>
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Nowadays, viscoelastic materials are widely used in industry, e.g. in aerospace and automotive. In many applications they are exposed to long-term loading conditions. In this work the classical Finite element approach mis substituted by a space-time model order reduction approach for solving nonlinear structural problems which are subjected to long-term loading. While Reduced Basis (RB) methods are often used to compress spatial information at given time instances, in our current approach each basis function of the RB gives the full time-dependent field information in a finite time interval. Reduced variables are obtained by projection of space-time local stationary conditions onto appropriate space–time test functions. This leads to a low-dimensional nonlinear system of equations. Furthermore, remarkable saving in terms of CPU time is obtained, due to the low number of required iteration for solving the system.
| PP1.005 | A Multiscale Moving Mesh Method for Phase Transitions  
Maria Wiebe, Christian Rohde |
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<td><strong>●</strong></td>
<td>Evolution of stress-induced phase transformations in crystalline solids depends critically on the dynamics of the corresponding particle lattice defects. For a macroscopic description with elastodynamical conservation laws, phase boundaries are represented as sharp interfaces. The end states of phase boundaries are determined in classical theories from a macroscopic algebraic coupling condition called kinetic relation. Since kinetic relations cannot always capture the effects of the lattice dynamics, we aim at replacing the macroscale kinetic relation by more precise mesoscale models. Following the achievements in a previous SimTech project we present a generalization of the moving mesh multiscale method of to the system case and several space dimensions and show numerical results. The presented method enables the usage of different mesoscale models via the concept of the interface solver and ensures a sharp resolution of the phase transition at the macroscale.</td>
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| PP1.006 | Simulation of Dynamic Processes in Polymer Systems Loaded with Magnetic Nanoparticles  
Patrick Kreissl, Nicolai Roth, Rudolf Weeber, Christian Holm |
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<td><strong>●</strong></td>
<td>Polymer gels and suspensions loaded with magnetic nanoparticles are smart materials whose shape, elasticity and rheological properties can be controlled dynamically using magnetic fields. This is of particular interest for biomedical applications such as artificial muscles and drug delivery, as biological matter is tolerant to magnetic fields. Particle-based simulations are a valuable tool for studying the materials since they are able to explicitly resolve the magnetic colloids embedded in them. In this contribution, we report on the deformation of magnetic gels in external fields and on the role of the gel’s architecture. One aspect which is sometimes hard to access experimentally is the nature of the coupling between the polymers and the magnetic nanoparticles. Simulations can help to clarify this, by studying the influence of different coupling mechanisms on experimentally accessible properties such as results from frequency-dependent measurements of the magnetic susceptibility.</td>
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| PP1.007 | Numerical Upscaling for Compressible Phase Field Flow  
Lukas Ostrowski |
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<td><strong>●</strong></td>
<td>We consider a diffuse interface approach to model compressible two phase flow. To be precise, we use a compressible Navier-Stokes-Allen-Cahn model. In many applications, microscopic effects can heavily influence the macroscopic dynamics of a system, for example in case of impingement of a droplet onto a rough surface. However, it can be prohibitive costly to resolve all microscopic structures in simulations. To overcome this issue homogenization and numerical upscaling techniques can be applied. In our contribution we present an approach for numerical upscaling of the compressible Navier-Stokes-Allen-Cahn model in vicinity of rough surfaces and discuss differences to the steady or incompressible case.</td>
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### PP1.008 Variational Multiphysics of Smart Functional Materials
**Daniel Vallicotti, Marc-André Keip**

Complex macro-phenomena in functional materials such as coupled multi-field effects require new modeling techniques accounting for microstructural mechanisms. Examples for material systems which need a multiscale modeling approach are piezoelectric as well as electro- and magnetostrictive materials. The multiple effects can reliably be described by multiscale approaches reducing the empiricism of purely macroscopic theories and by accounting for the evolution of microstructure via scale bridging techniques. We give an overview on our works on magneto-electro-mechanically coupled systems where we investigate the effects of composite micro-structures on the overall macroscopic material response. Focus is set on the treatment of multi-scale instability phenomena based on a stability analysis that accompanies the numerical solving procedure for both micro- and macroscopic instabilities. The advances of our recent work on homogenization of micro-magneto-mechanics are also outlined.

### PP1.009 Particle Mechanics and Microcontinuum Theories
**Sami Bidier, Wolfgang Ehlers**

Microcontinuum theories allow for a consideration of microstructural effects in a continuum mechanical approach, exemplarily by taking rigid or homogeneously deformable micro-elements (the micropolar and the micromorphic model, respectively) into account. However, their physical justification is not a priori given. Homogenisation strategies, as the one presented here, which links particle-based interaction quantities with microcontinuum stress states, supply this justification. The homogenisation is based on ensembles of particles forming a Representative Elementary Volume on the mesoscale. In order to demonstrate the applicability of the proposed averaging technique, localisation problems in bonded and unbonded granular media are studied using the Discrete-Element Method and a subsequent homogenisation of the microstructural information is performed. Results show the activation of the extended stress states in the localised zones and allow a comparison between existing models.

### PP1.010 Density Functional Theory as Bridge Between Statistical and Continuum Mechanics
**Philipp Rehner, Joachim Groß**

Modeling of interfaces is a challenge in classical fluid dynamics. To attain a thermodynamic consistent description of the interface, a method based on statistical mechanics, like molecular dynamics simulation, has to be used. However, these methods become far too costly on the time and length scales, that are of interest in most applications. We want to show, how density functional theory can be used to get a consistent description of bulk phases, as well as the phase boundaries. In sharp interface modeling, density functional theory can be used to dynamically determine surface tensions as well as mass and thermal resistivities, dependent on the state of the interface. If the functionals used are based on an equation of state, like PC-SAFT, all calculated properties are consistent with the properties of the bulk phases. In diffuse interface modeling, density functional theory can be used to calculate a
temperature and density dependent influence parameter from the equation of state.

**Computational Characterization of Soft Magneto-Electro-Mechanical Materials**
Matthias Rambausek, Marc-André Keip

Materials with magneto-electric (ME) coupling allow for, e.g., ME random access memories and electrical magnetic-field sensors. Since single-phase materials exhibit extremely weak coupling, ME composites become relevant. As an alternative to classical approaches based on multi-ferroics and hard-matter-based composites, we discuss new realizations of ME coupling with soft-matter composites. In comparison, such soft composites are easier to manufacture and have less expensive constituents. In order to assess the full potential of these promising soft ME composites one has to account for their micro-heterogeneous nature as well as for macroscopic magneto-electric coupling. Thus, in our contribution we present two scale simulations of prototypical magnetic-field sensor scenarios in two dimensions. Thereby we focus on the distinction between macro- and microscopic effects. In addition to that we also present a non-standard variational framework for macroscopic magnetoelectro-elasticity.

**CASSCF for Complex Molecules**
David Kreplin, Peter Knowles, Hans-Joachim Werner

Ab inito methods allow the quantum chemical investigation of molecular systems based only on the geometry and natural constants. They provide the computation of the energy and various other chemical and physical properties, up to experimental accuracy. The complete active space self-consistent-field (CASSCF) method enables the computation of the first-principle wavefunction for multi-configurational systems. It is necessary for the treatment of electronically excited states, transition metals, bond breaking and more. To construct the multi-configurational wavefunction, a selection of molecular orbitals is necessary, which reflects the physical behavior of the system. Post CASSCF methods are available and provide experimental accuracy. In our work, we improve the CASSCF method to make it more efficient for larger molecules and simplify the selection of the relevant orbitals. The methods are available in the quantum chemistry software package MOLPRO.

**Modeling Defects and Grain Boundaries Within the Amplitude Expansion of the Phase Field Crystal Model**
Marco Salvalaglio, Rainer Backofen, Ken Elder, Axel Voigt

The Phase-Field Crystal (PFC) approach describes the dynamics of local atomic probability density on diffusive time scales. It is restricted to relatively small systems as it requires fine spatial discretization. The Amplitude expansion of the PFC model (APFC) is a coarse-grained approach allowing for tackling larger systems. However, it has limitations on the quantitative description of material properties and on 3D systems. We present the realistic modeling of grain boundary morphologies between tilted/twisted and strained crystals by means of the APFC model. This is achieved through a Finite Element Method framework with advanced computational features and an extension of the model allowing
for the control over the energy of defects, grain boundaries, and interfaces. Typical planar and spherical grain boundaries are illustrated for different lattice symmetries, namely triangular/honeycomb in 2D as well as body-centered cubic and face-centered cubic in 3D.

| PP1.014 | **Optoelectronic Properties of Functionalized Diamondoids: Sensing DNA-Nucleotides**  
Chandra Shekar Sarap, Partovi-Azar Pouya, Frank Uhlig, Maria Fyta |
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<td>Diamondoids, the small nanometer-sized hydrogen-terminated hydrocarbon cages or diamond like with sp3 carbon, are complementary to sp² carbon systems such as graphene, carbon nanotubes, and fullerenes. Due to the unique molecular framework, these molecules have recently gained a lot of interest and possess high thermal stability, superior chemical resistance, and negative electron affinity which makes them to be used in electron emitting devices. Herein, we investigate the performance of functionalized diamondoids as a probe to sense DNA using first-principles based electronic structure simulations. We look at the optical properties of functionalized diamondoids interacting with the nucleotides by estimating the hydrogen bonding strengths and the corresponding charge transfer using time-dependent density functional theory (TDDFT). The studies are motivated by the high potential of diamond-based materials to be used in optoelectronic applications and as sensors for DNA detection.</td>
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| PP1.015 | **Comparison of Precipitate Interaction with Edge and Screw Type Dislocations via Molecular Dynamics**  
Dennis Rapp, Stephen Hocker, Siegfried Schmauder |
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<td>Using Molecular Dynamics shear tests, the interaction of dislocations with obstacles (nano-scale precipitates) in the Cu-Ag material system is investigated. By performing a parameter study in dependence of precipitate shape and size as well as dislocation character, the mechanisms of dislocation/ particle interaction were revealed for this system. For edge dislocations complex circumvention mechanisms such as the formation of dislocation loops or so-called double-jogs have been observed especially for spherical precipitates. The interaction for screw dislocations on the other hand is usually a complete circumvention enabled by the cross-slip mechanism, which is typical for screw dislocations. The misfit-dislocation configuration present at incoherent interface of the precipitates is found to be a major influence on the interaction mechanism, which in the end determines the critical stress needed to bypass an obstacle. This is a key value for determining the precipitation strengthening.</td>
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| PP1.016 | **Understanding Ion Dissociation and Association Mechanisms Using MD Simulations**  
|         | Anand Narayanan Krishnamoorthy, Christian Holm, Johannes Zeman |

We present a theoretical framework for co-solute and solvent effects on the chemical equilibrium for ion pair formation based on Kirkwood-Buff integrals. We show that ion pair formation or ion dissociation is favored with regard to a more pronounced co-solute accumulation around the corresponding ion state [1]. Also specific counterion condensation effects in different solvents is studied for alkali halide ions with model polyelectrolyte using atomistic MD simulations. Furthermore, we parameterized reactive forcefields (REAXFF) for acrylic based weak electrolytes to study the ion transport and diffusion process of dissociable groups with reference abinitio calculations and optimization of charge equilibration schemes [1]. The implications of our studies are useful in order to optimize the efficiency of electrolyte solutions in electrochemical applications.

| PP2.017 | **Interpolation of Potential Energy Surfaces using Gaussian Process Regression**  
Alexander Denzel, Johannes Kästner |
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<td>In this work we are combining methods of quantum mechanics with machine learning methods to find interesting geometries of molecules and other useful properties of chemical systems. One of the fundamental problems in theoretical chemistry is the steep scaling of the calculations that are necessary to determine the energy and its derivatives in a chemical system. We use machine learning methods like neural networks and Gaussian process regression (GPR) to interpolate between obtained energies. GPR is easy and fast to set up for a new system. Furthermore, formulated in a Bayesian setting, it has the capability of giving uncertainty measurements and the possibility of optimizing its parameters with e.g. the maximum likelihood method. We apply this method to interpolate several energy surfaces to do geometry optimization and reaction rate calculations that incorporate quantum mechanical tunneling with fewer electronic structure calculations and therefore, faster than before.</td>
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| PP2.018 | **Improvements of Instanton Theory to Simulate Atom Tunneling in Astrochemical Reactions**  
Johannes Kästner |
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<td>Instanton theory, based on Feynman path integrals, is increasingly used for accurate prediction of reaction rate constants. We present methodological improvements in several aspects: its accuracy close to the crossover temperature and its limit below that temperature, its convergence properties with the number of images, its temperature-dependence for bimolecular rate constants at low temperature, as well as its dependence on the quality of the potential. Some of these aspects were improved on by using a microcanonical formulation of instanton theory. We applied instanton theory to several reactions of astrochemical interest. Atom tunneling allows reactions to proceed at the cryogenic temperatures of the interstellar medium despite a reaction barrier. These help to explain the formation of water and of the first building blocks of life.</td>
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| PP2.019 | **Uncertainty Quantification for Compressible Flows and Aeroacoustics**  
Fabian Meyer, Andrea Beck, Jakob Dürrwächter, Thomas Kuhn, Claus-Dieter Munz, Christian Rohde |
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<td>Aeroacoustics studies the noise generated through pressure fluctuations in a flow field. In the automobile industry the main aeroacoustic noise sources of a car are the side mirrors and small cavities such as door gaps. The exact configuration of these objects and their physical environment are always, to some extent, subject to uncertainty. The aim of Uncertainty Quantification is to quantify the influence of uncertainty in the input parameters on numerical simulation results. In this contribution we present Multi-Level Monte Carlo and non-intrusive polynomial chaos methods to quantify and examine the influence of uncertain model parameters on the development of tonal noise. We discuss their advantages and disadvantages and present some numerical results obtained by both methods.</td>
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| PP2.020 | **Calculation of Reaction Rate Constants via Instanton Theory in the Microcanonical Ensemble**  
Andreas Loehle, Johannes Kästner |
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<td>The phenomenon of quantum tunneling is crucial in order to make accurate predictions for chemical reaction rates, particularly for those involving the transfer of light atoms such as hydrogen. One method to describe tunneling effects in large systems is the use of canonical instanton theory which allows the calculation of reactions rates at well defined temperatures. However, canonical instanton theory is fundamentally restricted to temperatures below the crossover temperature $T_c$. Additionally, it can be challenging to obtain instanton solutions at very low temperatures as well. An alternative approach to obtain thermal rates is provided by a microcanonical formulation of instanton theory which in principle is able to provide thermal rates at all temperatures. The objective is therefore to obtain microcanonical rates first in order to calculate thermal rates later while circumventing the existing limitations of using canonical instanton theory directly.</td>
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| PP2.021 | **Minimally Invasive Load-Balancing for Short-Range Molecular Dynamic with ESPResSo**  
Steffen Hirschmann, Dirk Pflüger, Colin W. Glass |
| For large-scale short-range molecular dynamics simulations with dynamically changing, heterogeneous particle distributions, flexible load balancing methods are mandatory to achieve good parallel efficiency. Designing and implementing such algorithms is complex, especially for existing applications which were not designed to support arbitrary domain decompositions. Here, we present our approach to incorporate general domain decompositions and dynamic re-balancing into the existing MD software ESPResSo in a minimally invasive way. It enables us to keep the whole range of physics algorithms in ESPResSo. We show results for heterogeneous short-range MD scenarios with a load balancer based on space-filling curve. They indicate that our approach is capable of reducing the imbalance amongst processes and the total runtime in simple and complex scenarios. Additionally, we show how these adaptions integrate into an overall concept of load balancing multi-physics simulations in ESPResSo. |
| PP2.022 | **Fitted Potential Energy Surfaces in Non-Redundant, Translationally and Rotationally Invariant Coordinate Systems**  
Sean McConnell, Johannes Kästner |
<p>| Potential energy surfaces fitted using machine learning methods have become popular as they reduce the time required to obtain a qualitatively accurate picture of the energy landscape of a molecule containing many degrees of freedom. We seek to use a fitted PES in the calculation of reaction rate constants using instanton theory, where knowledge of gradients and hessians is required at the different molecular configurations along the instanton path. If the input coordinates are cartesian, the learning algorithm must be trained to learn about the rotational and translational independence of the properties of interest. We propose the use of a coordinate system which is independent of any rotational or translational degrees of freedom. We have implemented two neural network algorithms to fit the potential energy surface of the reaction |</p>
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<th>Session</th>
<th>Title</th>
<th>Author</th>
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<tr>
<td>PP2.023</td>
<td>Isogeometric Analysis for Industrial Applications</td>
<td>Matthias Möller</td>
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<td>The EU-funded MOTOR project is developing simulation and optimisation</td>
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<td>tools that enable integrated design workflows for aircraft engines,</td>
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<td>water turbines, ship propellers, and screw compressors. Next to giving</td>
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<td>a brief project overview, we will present an isogeometric analysis-</td>
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<td>based (IgA) solver for compressible flows and its HPC implementation</td>
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<td>in the open-source software G+Smo. The solver makes use of meta-</td>
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<td>programming techniques to combine several efficient linear algebra</td>
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<td>backends with the fluid dynamics expression-template library G+Smo.</td>
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<td>Just-in time compilation is used to run the solver in heterogeneous</td>
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<td>environments. We will furthermore describe an isogeometric approach</td>
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<td>for creating analysis-suitable multi-patch parameterisations for</td>
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<td>rotary screw compressors thereby making use of elliptic grid generation</td>
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<td>techniques extended into the IgA framework.</td>
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<td>PP2.024</td>
<td>Calculation of Activity Coefficients for Solvent Mixtures from</td>
<td>Julia Gebhardt, Niels</td>
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<td>Molecular Dynamics Simulations</td>
<td>Hansen</td>
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<td>The calculation of free energy differences from molecular dynamics</td>
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<td>simulations gives access to thermophysical properties like binding</td>
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<td>free energies and activity coefficients. The method independent</td>
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<td>calculation of these properties can be of use in rational molecular</td>
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<td>design as well as force field validation. The twin-system approach</td>
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<td>for Enveloping Distribution Sampling has appeared to be a robust</td>
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<td>approach for determining relative free energy differences [1]. The</td>
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<td>method is applied to the calculation of activity coefficients of</td>
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<td>different solvent mixtures in this work. Particularly solvent</td>
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<td>mixtures with specific protein interaction characteristics are</td>
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<td>[1] Julia Gebhardt, Niels Hansen Calculation of binding affinities for</td>
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<td>linear alcohols to α-cyclodextrin by twin-system enveloping</td>
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<td>distribution sampling simulations. Fluid Phase Equilib., 422 (2016),</td>
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<td>PP2.025</td>
<td>Towards Realistic HPC Models of the Neuromuscular System</td>
<td>Aaron Krämer</td>
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<td>Within the “Digital Human” project we want to contribute to the grand</td>
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<td>vision of a virtual physiological human model, by developing a</td>
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<td>realistic model of the neuromuscular system. Due to the high complexity</td>
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<td>of the neuromuscular system, detailed multiscale computational models</td>
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<td>are indispensable, e.g. representing the chemo-electro-mechanical</td>
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<td>behaviour of the system or the global mechanics. To make progress</td>
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<td>towards a close-to-realistic model of the neuromuscular system we aim</td>
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<td>at a holistic revision of the physical, numerical and computational</td>
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<td>models at all scales. We adapt solution strategies of the discretized</td>
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<td>models to increase the discretization order and thus, reduce the</td>
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<td>computational effort. Additionally, we realised parallelization</td>
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<td>improvements and</td>
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performed scalability measurements to examine the main bottlenecks. The work is carried out using OpenCMISS, a code framework for developing computational modelling and visualisation software, particularly targeting bioengineering.

| PP2.026 | **Impact of Backbone Hydrogen Bonding and Inter-Domain Interactions for the Stability of Human Protein Pin1**  
Daniel Markthaler, Niels Hansen |
| A detailed understanding of protein stability is crucial for protein engineering as well as the denovo design of enzymes. In this project the effect of mutations in the protein backbone is investigated for the WW domain of human protein Pin1. This protein is well characterised experimentally, small enough to allow for substantial simulation time scales and representative for one of the main factors influencing protein stability, i.e. backbone hydrogen bonding. By systematically switching off or at least quantifying the major simulation-related inaccuracies that hamper the agreement with experimental data, it is aimed for linking a residual discrepancy between experiment and simulation to either force field inaccuracies or uncertainties in the experimental measurements. Another aspect of this project considers the inter-domain interaction between the WW domain and the PPIase domain of Pin1 by means of free energy calculations and Differential Scanning Calorimetry (DSC) experiments. |

| PP2.027 | **Fast and Accurate Characterization of Approximate Computing Designs on Heterogeneous Computer Architectures**  
Alexander Schöll, Claus Braun, Hans-Joachim Wunderlich |
| Approximate Computing (AC) trades off precision for efficiency gains with respect to power, energy, execution times, computational performance, and chip area. The characterization of such design parameters requires fast and accurate simulation methods that tackle AC as a multi-layer challenge with respect to interplays between software, hardware, and AC techniques. A major challenge is induced by additional parameters like the approximation error, error resilience and accuracy demands that increase the design space complexity. This poster presents a simulation method that exploits heterogeneous computer architectures for fast and accurate characterizations of AC designs. The underlying hardware simulations that generate timing, power, and energy results are accelerated by many-core GPUs, which allows significant runtime reductions. The characterization of two widely-used simulation tasks (Linear system solving, Linear programming) on AC hardware shows high result accuracy. |

| PP2.028 | **QM/MM Study of an Atom Tunneling in the Hydroxylation Process of Taurine/α-Ketoglutarate Dioxygenase (TauD)**  
Sonia Álvarez Barcia, Johannes Kästner |
| Enzymes of the class of α-ketoglutarate dependent dioxygenases (αKGDs) are vital in many biochemical processes, while details of their reaction mechanism remain poorly understood. This study focuses on one of the most studied αKGDs: the Taurine/α-ketoglutarate Dioxygenase (TauD). More concretely, we are interested in clarifying one of the key steps in the catalytic cycle of the αKGDs, the hydrogen atom transfer (HAT) process. We have studied the HAT |
process in TauD by QM/MM simulations. Analysis of the spin densities during the reaction demonstrates that a concerted mechanism takes place, where the H atom transfer happens simultaneously with the electron transfer from taurine to the Fe=O cofactor. In addition, we have found that the reaction is significantly enhanced by atom tunneling causing a KIE of about 60, which is in excellent agreement with the experimental value of about 58. These results influence our understanding of the whole class of αKGDs.

PP2.029 ESPResSo – A Flexible Simulation Package for Soft Matter, Biophysics and Process Engineering Research
Florian Weik, Christian Holm, Rudolf Weeber, Konrad Breitsprecher, Jonas Landsgesell, Kai Szuttor, Georg Rempfer

ESPResSo is a molecular dynamics software package primarily designed for fundamental and applied research in the field of soft and biological matter as well as in process engineering. A particular focus are applications on the nano and mesoscale, where the relevant energy scales are comparable to the thermal energy and Brownian motion may play an important role. The software is used by researchers world-wide and has been applied to study DNA in nanopores, membranes, hydrogels and other stimuli-responsive materials, microfluidics and many other systems. Through a combination of a parallelized simulation core written in C/C++ with a newly developed Python interface, ESPResSo provides a large flexibility. This is of particular interest for the development of new simulation techniques and protocols. Furthermore, through its Python interface, the software can be connected to other scientific packages. ESPResSo is being used for several projects in the SimTech Cluster of Excellence.

PP2.030 Visual Exploration of Memory Traces and Call Stacks
Patrick Gralka, Christoph Schulz, Guido Reina, Daniel Weiskopf, Thomas Ertl

In the case of simulation software for high-performance computers, node-level performance is amongst others an area of possible code optimizations. For such software, efficient memory usage and cache efficiency are important. Analyzing cache efficiency in high-level source code is not a trivial task, e.g. compiler optimizations obfuscate the intent of memory access patterns. We present a tool that gathers information on memory usage at machine-code level. It traces memory access instructions such as MOV*, as well as Call and Return statements, at runtime by instrumentation. A density-based scatter plot visualizes each atomic memory access from the traced instructions as a point representing memory address over time. Cache-inefficient or other typical memory access patterns are immediately visible. The call stack progression, which is reconstructed from the traced Call and Return instructions, is displayed as a flame graph that is used to relate memory accesses back to the source code.
**PP2.031 Charge me Slowly, I’m in a Hurry: Accelerating Charge/Discharge in Narrow Pores**  
Konrad Breitsprecher, Christian Holm, Svyatoslav Kondrat

Nanoporous supercapacitor have attracted much attention recently as green energy storage devices with remarkable cyclability, and high power and energy densities. However, their use in high frequency applications is limited by a relatively slow charging process. Here, I will focus on the physics and optimization of charge/discharge cycles in finite nanopores. We will see that step-voltage charging can be slow because the coions become trapped in narrow pores of supercapacitor electrodes. To avoid such trapping, a slow voltage-sweep charging is considered, which allows to accelerate the overall charging process substantially. However, we will demonstrate that a step-voltage, rather than sweeping, is preferable for fast discharging. Based on these results we will propose an optimal charge/discharge cycle.

**PP2.032 Modelling DNA Induced Current Modulations in Nanopores**  
Kai Szuttor, Florian Weik, Georg Rempfer, Christian Holm

We study the current modulation in nanopores caused by the presence of single DNA and Origami-DNA structures. We extend on results from molecular dynamics modelling approaches and describe the DNA on the continuum level. Solving the system of coupled differential equations (Diffusion advection equation for ion transport, Poisson-Boltzmann for electrostatics, Stokes for hydrodynamics) of the standard electrokinetic model, we are able to reproduce key experimental results of Keyser et al [1, 2].


**PP2.033 Influence of Atom-Tunneling and Ice Surfaces on the Reaction Rates of Interstellar Water Formation**  
Jan Meisner, Thanja Lamberts, Johannes Kästner

Atom tunneling plays a crucial role for reactions in cryogenic environments like in the interstellar medium. Reactions are assumed to be catalyzed heterogeneously by surfaces coated with water ice. The reaction of H2 with the OH radical is one of the most important routes of water formation in astrochemistry even though it possesses an activation energy of 24 kJ mol−1. We calculated the gas-phase reaction rate constants using semiclassical instanton theory on a fitted potential energy surface [1]. The results are compared to harmonic transition state theory (HTST) to quantify the impact of atom tunneling [1]. We also present the influence of an ice surface on the reaction and propose a new approach of mimicking a surface by modifying the rotational partition function. To calculate the reaction on the ice surface a QM/MM setup with a thoroughly benchmarked QM region was used. The importance of ice surfaces for reactivity in the interstellar medium is discussed [1].
<table>
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<tr>
<th>PP2.034</th>
<th>A Coarse-Grained Polarizable Force Field for the Ionic Liquid 1-Butyl-3-Methylimidazolium Hexafluorophosphate</th>
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<td>Johannes Zeman, Frank Uhlig, Jens Smiatek, Christian Holm</td>
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<td>We present a newly developed molecular dynamics force field for the ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate ([BMIm][PF6]) which combines a coarse-grained representation with the explicit treatment of dipolar electronic polarizability. Due to this combination, our model profits from the reduction of computational cost due to its coarse-grained representation while we expect it to be an improvement over non-polarizable models in situations where an explicit treatment of electronic polarizability might be crucial. This should for example be the case under confinement or at liquid/vapor interfaces. Furthermore, in contrast to models which treat polarization effects in a mean-field fashion, our force field is expected to be transferable with respect to its applicability in different dielectric environments. Here, we assess the force field in terms of its ability to reproduce thermodynamic key features, covering both static and dynamic bulk observables.</td>
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<th>PP2.035</th>
<th>Building Blocks of Proteins</th>
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<td>Catharina Zeil, Jürgen Pleiss, Lenz Lorenz</td>
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<td>Because of sheer statistics, evolution on the level of a complete protein is not effective. It has been suggested that protein evolution is limited to shorter sequence stretches. By analyzing three large protein families of different fold classes, sequence segments of 15 – 20 amino acid length were identified. By linking sequence segment pairs with a sequence identity of more than 50 %, a single connected network with 196518 nodes was formed. Links were found between sequence segments of the same protein, but also between sequence segments of different folds. The existence of a connected network indicates that evolution occurs on the level of these sequence segments by mutation and duplication. We call this principle the &quot;protein monad&quot;. The existence of the protein monad provides insight into the principles of structure, structure formation, and evolution of proteins and has relevance for the design of novel, not-yet-found or not-yet-born, proteins and protein-inspired molecules.</td>
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<th>PP2.036</th>
<th>Simulations of Protein Diffusion and Aggregation for Bioprocess Design and Optimization</th>
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<td></td>
<td>Valerio Ferrario, Jürgen Pleiss</td>
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<td>Improving the productivity of a bioprocess requires detailed understanding of the behavior of the biocatalyst under process conditions because high substrate concentrations, organic solvents or elevated temperature promote protein aggregation. Molecular dynamics simulations were applied to study diffusion and aggregation of Lipase B from Candida antarctica (CALB) in water and at high substrate concentrations. In solution, substrate, additives and solvent molecules compete for binding at the protein surface and thus modify protein interactions and aggregation behavior. Since the simulation of biocatalysts under process conditions provides insights into kinetic pathways of protein association as well as the molecular structure of aggregates, it is a valuable starting point for process engineering and enzyme design.</td>
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| PP2.037 | **Fault-Tolerant Numerical Methods**  
Mirco Altenbernd |
---|---|
Fault-tolerance is one of the major challenges towards extreme-scale computing. There is broad consensus that future leadership-class machines will exhibit a substantially reduced mean-time-between-failure. The resilience challenge can best be summarised that at scale, faults and failures are likely to become the norm rather than the exception: Any simulation run will be compromised without inclusion of resilience techniques into the software stack and system. The expected increase in the number of cores in particular will have a major impact. Therefore, we developed a hierarchical checkpoint system for multigrid solvers based on the Full Approximation Scheme to generate checkpoints with reduced memory usage, as well as an algorithm-based fault-tolerant multigrid scheme with respect to soft transient faults. In addition, we present a high-level C++ approach to manage local errors, asynchrony and faults with MPI which will integrate seamlessly with upcoming MPI-ULFM versions.

| PP2.038 | **AutoTuneTMP: C++ Runtime Template Metaprogramming for Auto-Tuned Astrophysics**  
David Pfander, Dirk Pflüger |
---|---|
Due to multiple levels of parallelism and complex memory hierarchies, maximizing performance on modern hardware platforms has become more and more difficult. Auto tuning techniques can address these challenges through compute kernels that automatically adjust to the underlying hardware platform. AutoTuneTMP is a C++-based auto tuning framework that uses just-in-time compilation to enable runtime-instantiable C++ templates. These templates provide data structures and algorithms that support the development of tunable compute kernels. We used AutoTuneTMP to accelerate an astrophysical application that simulates white star mergers in binary star systems. For an accurate, high-resolution discretization, this application requires excellent node-level performance. Our auto-tuned implementation of different fast multipole compute kernels achieves up to 30 % of the peak performance on an Intel Skylake platform. Similar results were observed on an Intel Knights Landing platform.

| PP2.039 | **Scalibility Studies and Implementation Details of a GPU-Accelerated SPH Method**  
Malte Schirwon |
---|---|
Direct Numerical Simulation of fluid flow in high-resolution imaged geometries of real porous materials is highly relevant in several fields, such as, carbon dioxide sequestration, geothermal energy generation and groundwater contamination remediation. One method commonly applied for DNS in these settings is quasi-incompressible Smoothed Particle Hydrodynamics (SPH). SPH is a meshless Lagrangian method, highly suitable for modelling complex geometries and flow at high Reynolds numbers. However, SPH requires high computational resources, especially in the simulation of large domains and leads to a very unstructured data structure. To overcome these difficulties, we have extended the highly optimized HOOMD-blue molecular dynamics software to
support the SPH method. Our implementation targets both CPUs and GPUs. We present details for an efficient GPU implementation, scalability studies of the SPH module for a variety of representative test cases and speed-ups over the CPU implementation.

**PP2.040**

**Minimally Invasive Integration of Tree-Structured Cartesian Grids in Existing Applications**

Michael Lahnert, Carsten Burstedde, Miriam Mehl

We present our approach for minimally invasive integration of dynamically-adaptive tree-structured grids at the example of the molecular dynamics (MD) simulation code ESPResSo. It includes an implementation of the Lattice-Boltzmann method (LBM) to subject a molecular ensemble to a background flow as well as a continuous representation of the electrokinetic equations. We port the grids of ESPResSo's physical subsystems to an extended version of p4est, a well-known and scalable library for tree-structured Cartesian grids. Our contribution to p4est allows simpler integration into existing applications. As not all grids are discretized in the same way, we use independent p4est instances for each algorithm and describe our approach for reducing communication in the coupling scheme. We show results and scalability tests for the individual components as well as for the integrated application on different hardware architectures.

**PP2.041**

**Simulation of Glycine Precursor Formation in the Interstellar Medium**

Max Markmeyer, Thanja Lamberts, Johannes Kästner

In the interstellar medium complex organic molecules can form even though the temperature and the density of molecules are very low. One such complex molecule is glycine, which is of special interest with respect to the origin of life. In this project we simulated the formation of the HOCO radical, that Woon suggested as a precursor to Glycine. In difference to Rimola, who investigated the HOCO formation by combination of CO and OH, we simulated its formation by hydrogen abstraction from formic acid. The reaction was simulated with different astrochemically relevant radicals (OH, NH₂, hydrogen atoms). Due to the low temperatures in the interstellar medium tunneling plays a major role for the reactions and the reaction rate constants were calculated with the instanton method.

**PP2.042**

**Assessing Entropy Scaling of the Viscosity of Mixtures Using Molecular Simulations**

Matthias Fischer, Oliver Lötgering-Lin, Joachim Groß

Reliable predictions and correlations of transport properties of mixtures, such as viscosity $\eta$ are important prerequisites for process design. Rosenfeld suggested that the reduced viscosity $\eta^r$ is a function of residual entropy $s_{res}$ only. The aim of this work is to give an assessment of entropy scaling for mixtures. We consider binary mixtures of LJ-fluids with differing $\epsilon$ and $\sigma$ parameters and a non-ideal mixture of two identical LJ-fluids. We calculated $\eta$ in equilibrium MD simulations and used Chapman-Enskog viscosity as a reference for defining $\eta^r$. $s_{res}$ was determined from Grand-Canonical Monte Carlo simulations. The
Reduced viscosities of all considered model mixtures show a universal dependency on $S_{res}$. These results could be used to develop a general correlation for all LJ mixtures, without the need of introducing further parameters. The new correlation approach shows excellent results for all considered real mixtures.

### PP2.043

**Potential Energy Surface Interpolation with Neural Networks**  
April Cooper, Johannes Kästner

A correct description of the potential energy surface (PES) is crucial to many simulation applications. However, obtaining reliable information on the PES and its first and second derivatives becomes very time consuming if several pieces of information are needed. Therefore, the interpolation of the PES with the help of artificial neural networks can lead to a significant speedup of computer simulations, which allows for the simulation of complex or large systems with an affordable computational effort. In order to show the capabilities of this simulation approach we calculated reaction rate constants for the reaction $\text{CH}_3\text{OH}+\text{H} \rightarrow \text{CH}_2\text{OH}+\text{H}_2$ with the instanton method on a PES fitted to high quality energy, gradient and Hessian values by neural networks. We further show that potential surfaces fitted by neural networks can be used in molecular dynamics simulations to describe the interactions of water molecules.

### PP2.044

**Modeling and Prediction of Supramolecular Complexes for the Design of Novel Material**  
Jörg Baz, Niels Hansen

Functional organic materials composed of dye-based molecules have fascinating optical and mechanical properties. These novel materials are of increasing importance for many high-technology applications. Perylene di-imide derivatives (PDIs) emerged as a prototype class of molecules for the elucidation of the transition from monomeric to bulk materials via the supramolecular state [1, 2]. Their self-assembly into complex structures is determined by size and shape of the monomeric unit, system composition and thermodynamic boundary conditions. In this project the free energy for the formation of dimers and higher aggregates are calculated for prototypical molecular building blocks carrying different functional groups in different solvent environments using molecular dynamics free-energy simulations based on force fields inherited from the area of biomolecular simulations.

### PP3.045

**An Extended Hill-type Muscle Model with Robust Routing Capabilities for Active Human Body Models**  
Christian Kleinbach, Jörg Fehr, Oleksandr Martynenko, Syn Schmitt

In the field of automotive safety Human Body Models are beginning to replace traditional crash test dummies as surrogate models for the occupants in crash simulations. Especially in low-G scenarios they can replicate the human behaviour much better than mechanical dummies. As passive safety systems are technically mature, the focus has shifted to active safety systems that act prior to a crash to mitigate or prevent possible impacts. Thus, the need for simulations of low-G scenarios will increase shortly. The introduction of autonomous vehicles will further increase the demand. One important aspect in modeling the human behaviour in low-G scenarios is muscle activity. This includes modeling muscle and tendon dynamics, correct routing of muscles around joints and activation dynamics. An extended Hill-type muscle model for the finite element software LS-DYNA is presented including two robust methods for muscle routing. The source code of the material model is available as open source.

### PP3.046

**Non-Intrusive Model Reduction with Machine Learning**  
Dennis Grunert, Kevin Carlberg, Jörg Fehr

Introducing model reduction usually involves changing existing simulation code at many places which is either cumbersome or not possible in case of closed-source software. We present a nonintrusive way to apply model reduction based upon arbitrary projection bases to any black box simulation code which provides only minimal access. Knowing the structure of the differential equation involved, we learn unknown functions of it with machine learning methods after projecting the data to a lower-dimensional space. Only an interface to the simulation code is needed to query the unknown function at arbitrary sample points. Since only reduced quantities are learned, the method is applicable for large systems. We present results of reducing, e.g., the 1D Burgers equation with Galerkin and Least-squares Petrov-Galerkin reduction inside a modular Matlab framework. The reduction basis is generated, e.g., from fullorder snapshots with POD.

### PP3.047

**Reducing the Influence of Transient Flow for Improved Wellhead Protection: An Engineered Optimal Pumping-Injection Management Solution**  
Abelardo Rodriguez Pretelin, Wolfgang Nowak

During Wellhead Protection Area delineation (WHPA) most engineering solutions assume that groundwater flow is at steady-state. However, nature is transient. Among the natural and anthropogenic causes triggering changes in well catchments, transient pumping rates are one of the most influential factors. Hence, in view of its high influence, we hypothesize that an optimized and dynamic adaptive pumping-injection management scheme can counter natural transient behavior, so that WHPA defined under steady-state assumption are made robust against nature transiency. Here we present an engineered pumping management scheme that reduces transient influence while considering additional management issues in well protection. To this end, we apply a multiobjective optimization (MOO) approach in order to find a compromise.
solution between three objectives: 1) to minimize groundwater abstraction from outside of a given WHPA, 2) to maximize groundwater supply and 3) to minimize the involved costs.

**PP3.048 Networked Control Systems with Advanced Interfaces Between Control and Communication**  
Steffen Linsenmayer, Frank Allgöwer

Networked Control Systems are control systems where at least one of the feedback links is replaced by a shared communication medium. Thus, the resulting problems lie in the intersecting area of control and communication theory which explains the need for interfaces between those domains. One commonly used approach is to compute new control actions with a periodic sampling time while the network is modeled by the fact that not all messages are delivered in time and thus some messages are lost. Recently a new model for such a loss process, based on the concept of weakly hard real-time constraints, was suggested that still allows to guarantee system theoretic properties. This poster discusses the problem of stabilizing a linear plant with such a network model. Furthermore, an alternative approach will be suggested where the decision about the network traffic is already made in the sampling mechanism such that the resulting shaped traffic receives better guarantees from the network.

**PP3.049 An Experiment on Vision Based Indoor Localization**  
Ehsan Sharafian Ardakani, Henrik Ebel, Peter Eberhard

To have a precise control on mobile robots, an accurate localization system is required. Here, a vision based indoor multiagents localization system is investigated. Hence, two methods, image segmentation and point feature matching techniques are implemented to detect the position of mobile robots. Due to low speed mobile robots, just a single low quality camera is utilized. These methods are developed in Matlab and the ARToolkit augmented reality software and the experimental results are compared. Based on the localization system, an experimental setup to do fully distributed control is installed. In this setup, communication is facilitated by the robot operating system (ROS). The proposed schemes are carefully and successfully tested and the results show that the position and orientation of mobile robots are obtained with high accuracy.

**PP3.050 Sampling Strategies in Stability Analysis of Uncertain Milling Processes**  
Dominik Hamann, Peter Eberhard

In machining processes, stability lobe diagrams are in focus, where the region of stable operating points -- the technological parameters spindle speed and axial immersion -- is depicted. Using these, engineers in manufacturing are able to identify suitable parameters resulting in efficient and stable processes. Stability analysis of periodic, time-delayed differential equations, modeling surface regeneration, results in an implicit calculation of the stability limit, where the critical eigenvalue of the time-discretized system is located at the unit circle in the complex plane. Considering varying workpiece dynamics or parameter uncertainty, the computational effort gets hardly manageable, thus,
sophisticated sampling strategies are mandatory. The applied sampling strategies have to deal with non-monotonicity and non-smoothness of the critical eigenvalue. Furthermore, calculation schemes have to provide necessary information for intended uncertainty analysis based on the sampled data.

**PP3.051**  
*Towards a Stable and Fast Dynamic Skeletal Muscle Model*  
Mylena Mordhorst, Bernard Haasdonk, Oliver Röhrle

Forward simulations of three-dimensional, continuum-mechanical skeletal muscle models are computationally demanding and expensive. To adequately represent the muscles' mechanical behaviour, a fully dynamic modelling framework based on the theory of finite hyperelasticity, which accounts for the highly nonlinear, anisotropic, viscoelastic and incompressible material behaviour, needs to be established. Discretisation of the governing equations yields a nonlinear second-order differential algebraic equation (DAE) system, which represents a challenge for solution strategies as well as for the application of model order reduction techniques. In this contribution, we will compare different solution strategies (DAE index reduction, different solvers) as well as the performance of reduced order models obtained by means of Galerkin and Petrov-Galerkin projection using different projection and test spaces.

**PP3.052**  
*On Local Incremental Stabilizability and its Application to Model Predictive Control*  
Johannes Köhler

We present the system property “Local Incremental Stabilizability”. We characterize this system property in terms of local incremental Lyapunov functions. Furthermore, we show sufficient conditions for this system property based on the linearization of the nonlinear system dynamics and highlight some connections to the theory regarding linear parameter varying (LPV) systems. Furthermore, we highlight potential applications of this system property in Model Predictive Control. In particular, we illustrate how this property can be used for reference tracking and robust design in the context of predictive control. We believe that this property is a suitable tool to bridge the gap between linear and nonlinear system theory and correspondingly between linear and nonlinear control theory. In particular, this property serves as an extension to stabilizability in the context of nonlinear system dynamics. We illustrate the practicality of this system property with numerical examples.

**PP3.053**  
*Improving a Flexible Robot Model Using a Nonlinear Observer*  
Fatemeh Ansarieshlaghi, Peter Eberhard

Lightweight robots are highly interesting for their advantages such as saving energy with a smaller actuator or requiring less material. These robots are inherently flexible and this flexibility should be taken into account for modeling and controlling. The difficulty of designing a nonlinear controller for high flexibility is increased when the controller does not have any direct measurement of the end-effector position and flexible states. To overcome this problem, an observer to estimate the states is required. Hence, a nonlinear high gain observer is designed and implemented on the lambda robot. Experimental results of the designed observer show that the lambda robot does not behave...
as well as the model. Therefore, the model is updated by observing the system behavior and comparing it with the experiment. Measurement results using the improved model show the maximum end-effector tracking error is drastically decreased for the linear and nonlinear trajectories with high speed motion.

PP3.054

A Direct Synthesis Framework for Networked Control Systems
Christian A. Rösinger, Carsten W. Scherer

We introduce a framework to synthesize block-diagonal $H_{\infty}$-controllers with a parametric and a block-triangular dynamic component by convex optimization. This is motivated by a recent $H_{\infty}$-design approach for systems with delayed interconnections that are structured according to a strongly-connected communication graph. Our framework allows the extension to controller synthesis for more complex interconnections described by multiple strongly-connected graphs that are themselves coupled through a nested delay structure. In particular, we give a precise classification of all tractable structures by our framework and demonstrate the flexibility of the design framework by means of a vehicle platoon simulation with different controller communication scenarios.

PP3.055

What Technical Phenomena are Relevant when Designing the Optimal Energy Storage Mix?
Jannik Haas, Wolfgang Nowak

Energy storage systems are widely envisioned as a structural solution for the massive integration of renewable energy systems, as they can provide operational flexibility and shift energy to times with lower availability of water, sun, and wind. For planning the investment and operation of storage systems, different techniques are commonly used, ranging from simple control strategies to optimal control and mathematical optimization. Here, we present an optimization for finding the optimal storage mix. It decides about the location, type, and capacity of storage, and it plans the least-cost operation while satisfying a set of technical constraints (energy balance, reserves, autonomy). When applying to a real power system (1 representative year), this results in about 10 million decision variables and even more constraints. To tackle computing times, we perform a phenomenological model reduction by analyzing how the equations affect the final decisions and total costs.

PP3.056

Model Order Reduction for the Monodomain Reaction-Diffusion Equation in Neuro-Muscular System
Nehzat Emamy, Pascal Litty, Miriam Mehl, Thomas Klotz, Oliver Röhrle

The neuro-muscular system is a complex multiscale coupled system, for which realistic simulations are extremely computationally demanding. The most challenging part of a chemo-electromechanical model of a skeletal muscle tissue is the monodomain reaction-diffusion equation. The equation comprises microscopic reactions existing at the cell membrane and diffusion of the action potentials along 1D muscle fibres. In order to save computational resources and use HPC clusters more efficiently, we study the feasibility of applying model order reduction techniques (MOR) to the monodomain equation. Our goal is to use a smart accurate combination of the reduced and full model simulations. Applying the proper orthogonal decomposition (POD) to reduce the monodomain
equation saves us a factor of 2 in the computation time. Further speedup is expected by using the Greedy-POD and discrete empirical interpolation method (DEIM) for approximating the nonlinear reaction terms.

| PP3.057 | **Statistical Data-Driven Model Selection under Computational Time Constraints: Application to River Engineering**  
Sergey Oladyshkin, Anneli Guthke, Farid Mohammadi, Rebekka Kopmann, Wolfgang Nowak |
|---------|---------------------------------------------------------------------------------------------------|

A suitable representation of hydro-morphodynamic processes is crucial for successful river management. To predict sediment transport and river bed evolution, a variety of empirical formulas can be plugged into river models and modelers lack objective guidance of how to select the most appropriate one. Such guidance can be provided by the Bayesian model selection (BMS) framework. Its applicability is however limited by high computational costs. To transfer it to computationally expensive river modeling tasks, we propose to combine BMS with model reduction via the arbitrary Polynomial Chaos Expansion. Despite iterative refinement of the reduced model, it needs to be acknowledged that they are only approximations of the models. We, therefore, introduce a novel correction factor in BMS, yielding a model ranking that is more representative of the full complexity models. We demonstrate our proposed approach on a case study for a stretch of the Rhine river.

| PP3.058 | **Adaptive Model Predictive Control**  
Matthias Lorenzen, Frank Allgöwer |
|---------|----------------------------------------------------------------------------------|

Adaptive control for constrained, linear systems is addressed and a framework based on Model Predictive Control (MPC) and set-membership system identification is presented. The work introduces a computationally tractable solution which uses observations of past state and input trajectories to update the model and improve control performance while maintaining guaranteed constraint satisfaction and recursive feasibility. The developed approach is applied to a stabilizing MPC scheme and depending on the cost function, finite gain stability or practical stability under persistent, additive disturbance is proved. A numerical example and brief comparison with non-adaptive MPC is provided.

| PP3.059 | **Simulating Non-Fickian Transport across Péclet Regimes by Doing Lévy Flights in the Rank Space of Velocity**  
Sebastian Most, Wolfgang Nowak, Marco Dentz, Branko Bijeljic, Diogo Bolster |
|---------|--------------------------------------------------------------------------------|

Transport in real porous media shows non-Fickian characteristics. This leads to skewed distributions of particle arrival times. The skewness is triggered by particles' memory of velocity that persists over a characteristic length. Capturing process memory is essential to represent non-Fickianity thoroughly. Recent methods use transitions matrices to parameterize memory which is then solely valid for this single Péclet regime. The method we propose overcomes three common drawbacks:

1) We simulate transport without restrictions in transition length.
2) We parameterize our CTRW without requiring a transport simulation.
| 3) | Our parameterization scales across Péclet regimes. We do so by sampling the pore-scale velocity so that particles keep their velocity over a certain spatial scale; the correlation length. We explicitly model memory including the evolution and decay of non-Fickianity, so it extends from local via pre-asymptotic to asymptotic scales. |
| PP3.060 | **Coarse-Graining on Graphs via Large Deviations**  
Bastian Hilder  
We introduce a new generalisation of the relative Fisher Information for Markov processes on discrete state spaces, and prove an inequality which connects this with relative entropy and large deviation rate functional. We use this inequality to study qualitative and quantitative coarse-graining problems for jump processes on discrete spaces. |
| PP3.061 | **Local Discourse Norms and Dual Process Decisions in an Opinion Dynamics Model**  
Malte Heckelen  
Depending on parameterization, most Bounded Confidence models lead either to complete consensus or complete fragmentation of the opinion space. Noise terms are normally introduced to achieve more realistic opinion dynamics. While this produces the desired results, it doesn't lend itself easily to a social scientific interpretation. Dual process models from Persuasion Studies and Sociology in contrast use momentary energy and association reinforcement to explain why an individual would “choose” to process messages with biases or behave according to norms instead of devising new solutions. This opinion dynamics model implements these micro-assumptions to see if they can be linked to the macro dynamics observed in previous Bounded Confidence models. The analysis will contrast the outputs of a simple Bounded Confidence Model with more complex extensions up until the final model and investigate dependencies on parameters such as network type. Preliminary results will be presented. |
| PP3.062 | **Deep Recurrent Gaussian Process with Variational Sparse Spectrum Approximation**  
Roman Föll, Bernard Haasdonk, Markus Hanselmann, Holger Ulmer  
Modeling sequential data has become more and more important in practice. Some applications are autonomous driving, virtual sensors and weather forecasting. To model such systems so called recurrent models are used. In this article we introduce two new Deep Recurrent Gaussian Process (DRGP) models based on the Sparse Spectrum Gaussian Process (SSGP) and the improved variational version called Variational Sparse Spectrum Gaussian Process (VSSGP). We follow the recurrent structure given by an existing DRGP based on a specific sparse Nyström approximation. Therefore, we also variationally integrate out the input-space and hence can propagate uncertainty through the layers. We can show that for the resulting lower bound an optimal variational distribution exists. Training is realized through optimizing the variational lower bound. We improve over current state of the art methods in prediction accuracy for experimental data-sets used for their evaluation. |
| PP4.063 | **Passivity-Based Ensemble Control for Cell Cycle Synchronization**  
| Karsten Kuritz, Frank Allgöwer, Wolfgang Halter |

We investigate the problem of synchronizing a population of cellular oscillators in their cell cycle. Restrictions on the observability and controllability of the population imposed by the nature of cell biology give rise to an ensemble control problem specified by finding a broadcast input based on the distribution of the population. We solve the problem by a passivity based control law which we derive from the reduced phase model representation of the population and the aim of sending the norm of the first circular moment to one. Furthermore, we present conditions on the phase response curve and circular moments of the population which are sufficient for synchronizing a population of cellular oscillators.

| PP4.064 | **Molecular Dynamics Simulations for the Detection of Unfolding Pathways and Stable Conformations of DNA Structures**  
| Ewa Anna Oprzeska-Zingrebe |

In nature, a wide range of biological processes, such as transcription termination or intermolecular binding, is dependent on the formation of specific DNA secondary and tertiary structures. These structures can be both stabilized or destabilized by osmolytes, coexisting with nucleic acids in the cellular environment. In our study, we investigate a simple 7-bp DNA hairpin with the sequence d(GCGAAGC) in the presence of varying concentrations of urea. The interaction between DNA and urea has been analysed according to Kirkwood-Buff theory. We implemented local/bulk partitioning model, complemented by the analysis of preferential hydration and preferential binding, to get insight into the distribution of the cosolute in the vicinity of the DNA surface. The free energy landscape of unfolding has been approached via Metadynamics upon the addition of a bias potential. This study allows us to get a more comprehensive understanding of the stability of DNA structures in the presence of urea.

| PP4.065 | **Poisson-Boltzmann Cell Model for Swelling of Macroscopic Polymer Gels**  
| Jonas Landsgesell, Christian Holm, Patrick Kreissl, Georg Rempfer, Florian Weik, Kai Szuttor |

Here we want to present the newly created Poisson-Boltzmann cell under tension model which allows the prediction of the swelling equilibrium of charged polyelectrolyte gels. At high charge fractions the Katchalsky model breaks down since the electrostatic energy functional makes use of the Debye-Hückel approximation and therefore a linearization of the PB equation. Solving numerically the PB cell model in the presence of salt we are able to obtain pressure curves which do not seem to become unphysical even for strongly charged gels.
Tracking Temporal Derivatives with a Genetic Network
Wolfgang Halter, Frank Allgöwer

Biological counterparts of differential operators are not only likely to exist in natural systems but also desirable to realize as modules in synthetic biology in order to realize internal controllers and optimizers. Therefore, we present a genetic regulatory network where its output concentration is approximately proportional to the temporal derivative of the input concentration. We synthesize the differentiator module by combining genetic regulatory parts realizing basic input/output functions such as a gain, integrator and signal difference. The resulting two-gene-network approximates the transfer function of a differential operator with additional low-pass filter. After several in-silico validations, a biological representation if this network was designed and genetically engineered as a proof of concept. This network was tested and validated in a cell-free transcription and translation platform.

From the Single Cell to the Cell Population
Stefan Engblom

I will present a newly developed computational framework designed specifically for the modeling of populations of living cells [4]. The framework is built around transparent assumptions, is very flexible, and has been designed from the very beginning with computational scalability in mind. The main applications are found in the study of embryo development, in wound healing processes, and in tumor models. The computational challenge is to bridge the vast scale separation inherent with these types of applications, and to provide for computational efficiency enough that the model can be effectively parameterized. In particular, I propose to couple the population-level description with single cell models described within the general umbrella of stochastic reaction-diffusion processes [1,2,3]. Examples in pattern formation, tumor modeling [4], and in the function of firing neurons will be used to highlight the overall framework.

| PP4.068 | **Pneumatic Muscle Spring Units: Designing Bioinspired Actuators Mimicking the Human Motion Apparatus**  
Simon Wolfen, Syn Schmitt |
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<td>In the last decades, research and development in science and industry developed a considerable amount of actuators. In complex technical systems, actuators with a high range of actuation and linear behavior e.g. electrical drives, dominate almost every field of application. In biological motion systems, on the contrary, the activation range of biological actuators (muscles) is limited and their behavior is nonlinear. However, the biological motion apparatus in total has excellent active and passive properties to perform precise movement. This raises the question how can we add biological actuator properties to artificial actuators? In this contribution, a combination of active and passive elements, according to the biological model, is investigated which enables the transfer of the biological properties to the field of robotics. It includes not only the single actuator itself, but rather extends the actuation concept to the actuator placement and arrangement.</td>
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| PP4.069 | **Modelling the Adaptation of Skeletal Muscles in Response to Isometric Exercise**  
Ekin Altan, Leonardo Gizzi, Sergey Oladyshkin, Oliver Röhrle |
| In this study, a computational model describing the adaptation of skeletal muscles in response to isometric exercise is used to investigate the corresponding neural adaptation mechanisms. A systematic review of the experimental studies on isometric unilateral knee extension exercise was performed. Data on the training regime and changes in maximal voluntary contraction (MVC) were extracted. A global sensitivity analysis was performed on the extracted data to investigate which parameters related to the training regime influence the improvement in MVC and to what extent. A motor unit (MU) recruitment model that generates force upon the summation of individual motor unit firings was used to compute the MVC. The properties of the MUs were altered according to what is known about exercise-induced neural adaptation to match the change in MVC for a given training regime. |
| PP4.070 | **Data Reconstruction from Electromyographic Signals in Biomechanics**  
Anna Rörich |
| Electromyographic (EMG) signals are used to examine the functionality of skeletal muscle and thus play an important role in understanding and treating neuromuscular dysfunctions. There are two ways of measuring EMG signals – intracellular, where needle electrodes are injected into the muscle, or non-invasive at the skin surface. The latter has the disadvantage that only the superposition of the electrical signals of multiple muscle fibers can be recorded. To overcome this drawback of surface EMG data, we need to “invert” the chemo-electro-mechanical muscle model which describes the excitation of muscle fibers and the propagation of electrical signals through the surrounding tissue. This leads to an inverse problem which can be treated as a regularized optimization problem or through a Bayesian approach to fit computed EMG signals to measurements. We study the applicability and behavior of both methods where the Bayesian approach has the advantage to allow for a priori error analysis. |
| PP4.071 | **Numerical Analysis of Multi-Dimensional Models for Network Flow in Biological Systems**  
Tobias Koeppl, Paolo Zunino, Barbara Wohlmuth, Ettore Vidotto |
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<td>Network structures can be detected in almost every biological system, since they are often responsible for the transport of fluids, nutrients or oxygen. One way to obtain a realistic model for such transport processes is based on a decomposition approach. Thereby, the network structure is separated from the surrounding medium and different models are assigned to both domains. Quite often the surrounding medium (e.g. tissue or soil) can be considered as a three-dimensional (3D) porous medium. In order to decrease computational costs while maintaining a certain degree of accuracy, flow and transport processes within the networks are modeled by one-dimensional (1D) PDE-systems. On this poster, we present a numerical analysis of PDE systems arising in the context of this model concept. In particular, it is investigated how the 1D line source terms and averaging operators affect the convergence behavior of standard finite element methods.</td>
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| PP4.072 | **Spatiotemporally Developing Layers of TRAIL-Resistant Cells Shield TRAIL-Hypersensitive Cells Within Multicellular Tumor Spheroids**  
Daniela Stöhr, Karsten Kuritz, Daniela Maichl, Tobias Beigl, Beate Budai, Jens O. Schmid, Thomas E. Mürdter, Roland E. Kontermann, Peter Scheurich, Nadine Pollak, Markus Rehm |
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<td>Tumor cell populations can show considerable heterogeneity in their sensitivity to cell death inducing anti-cancer agents. Here, we studied the susceptibility of multicellular tumor spheroids (MCTS) to 2nd generation TRAIL receptor agonists and observed that pronounced, spatially coordinated response heterogeneities manifest within spheroidal microenvironments: In MCTS grown from genetically identical cells, TRAIL-resistant subpopulations with low TRAIL receptor (TRAILR) expression develop and form layers that enclose and protect TRAIL-hypersensitive cells with high TRAILR2 expression, thereby leading to an overall increased treatment resistance. Interestingly, by using Cyclooxygenase II inhibitors we could achieve an upregulation of TRAILR2 and sensitization of the MCTS to TRAIL. Furthermore, data acquired during this project were used to generate a tumor growth model and to perform in silico simulation of spheroids using single cell data obtained by flow cytometry.</td>
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| PP4.073 | **Cell Population Dynamics During Apoptotic Treatment**  
|         | Dirke Imig |
|         | TNF-related apoptosis-inducing ligand (TRAIL) causes programmed cell death in cancer cells. Here, experimental results concerning cell populations stimulated with a second generation TRAIL variant are analyzed with help of an individual-based modeling framework. Model simulations predict a shift in caspase-8 distribution to be of capital importance for a transient insensitivity against TRAIL. Furthermore, it becomes clear that consideration of inheritance is crucial for understanding longterm responses. Interestingly, the comparison of data and simulations reveals differences referring to cell cycle dependence of death patterns. Hence, a phenomenological model is developed in order to verify possible connections between cell cycle and apoptosis. The analysis gives insights into mechanisms of cell death progression during the cell cycle. The presented results are important steps for the improvement of a predictive model with the objective of optimizing TRAIL-based cancer therapies. |

| PP4.074 | **Nucleotide-Specific Electronic Signals from Functionalized Nanopores**  
|         | Frank Maier, Ganesh Sivaraman, Maria Fyta |
|         | It has been shown, that nanopores can be used to build high-throughput DNA sequencing devices. Electronic tunneling signals are used as a fingerprint to differentiate the nucleobases. To enhance these signals, functionalized nanopores have been proposed. Previous work showed that DNA nucleobases show a specific binding to diamondoids which can assume a variety of sizes, have tunable optoelectronic properties, and can be selectively modified. We perform QM-calculations within the density functional theory (DFT) approach together with the non-equilibrium Green's function (NEGF) formalism to further investigate the properties of gold-electrodes modified with diamondoids, which are placed within a nanopore. For this, the electronic conductance across the nanopores and their sensitivity is assessed. We were able to show that this electronic transmission is nucleotide-specific and can be used to also identify modifications in the nucleotides, such as mutations and epigenetic markers. |

| PP4.075 | **Application-Driven Model Reduction for Multi-Component Porous-Media Models in a Biomechanical Context**  
<p>|         | Davina Fink, Arndt Wagner, Wolfgang Ehlers |
|         | Due to technological developments, computational simulations have a tremendous impact in many scientific fields. Considering biomechanical issues, it is desirable to gain a deeper understanding of the complex processes in the human body or to provide information for surgical interventions. Simulating such processes, a detailed knowledge about the inner structure of the materials is essential. This work deals with biological materials exhibiting a porous microstructure using a macroscopic continuum-mechanical modelling approach where the complex inner structure is regarded in a multi-component manner by means of the Theory of Porous Media. Furthermore, the FEM is used to approximate the solution of the set of coupled partial differential equations. However, a use of the simulation during clinical routines is usually not feasible due to high computation times. Therefore, model reduction methods (POD combined with DEIM) are applied in an application-driven way on the global FE equation. |</p>
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<td>PP4.076</td>
<td>Towards Investigating Aortic Valve’s Extra Cellular Matrix Remodelling from Cardiomyopathic Hearts</td>
<td>Sergio Morales, Oliver Röhrle</td>
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<td>To investigate the factors linking the destructive remodelling processes of an aortic valve’s (AV’s) extra-cellular matrix with ventricular diseases, a 3-D finite element model of the human AV is constructed. As patient-specific scenarios play a key role, the AV geometries are obtained through geometry extraction by different image segmentation approaches implemented on medical imaging data. Along with a suitable material model, physiologically accurate boundary conditions are implemented, recreating a palette of case-specific configurations where the bending and tensile stretches suffered by the cusps along the heart cycle are reproduced; giving an insight of the dynamics and the stress-stretch distribution of the main valve components at relevant stages of the valve’s opening and closing functions.</td>
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<td>P4.077</td>
<td>Continuum-Mechanical Metastases Model for Proliferation and Atrophy with Embedded Experimental Data</td>
<td>Patrick Schröder, Arndt Wagner, Daniela Stöhr, Markus Rehm, Wolfgang Ehlers</td>
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<td>The formation of vascularised metastases starts with the extravasation of cancer cells from the blood-vessel system into the tissue. Therein, the cancer cells proliferate while nutrients are consumed. To sustain the ongoing proliferation and basal reactions, vascular-growth factors are released inducing blood-vessel growth. The resulting vascularised metastases crucially affect the surrounding tissue. Therefore, a therapeutic agent is infused into the extracellular space of the tissue during metastases treatment. The applied therapeutic may then trigger the cell death of the metastases. These processes are described in a continuum-mechanical model based on the Theory of Porous Media. Therein, the proliferation as well as the cell death are described via mass production terms allowing to adjust the numerical simulations to lung-cancer experiments.</td>
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<td>PP4.078</td>
<td>Evaluating the Effects of Measurement Noise on the Inference of Biological Regulatory Networks Using Modular Response Analysis</td>
<td>Caterina Thomaseth, Dirk Fey, Tapesh Santra, Oleksii Rukhlenko, Nicole Radde, Boris Kholodenko</td>
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<td>Modular Response Analysis is a mathematical framework, which allows to unravel the topology of intracellular regulatory networks. MRA is widely used in systems biology, and relies on steady state measurements, like Western blot data, known to be quite noisy. The estimation of network interactions requires the solution of a reverse problem, which may be unstable with respect to noisy data. In this study we investigate how errors affect network inference using MRA and its robustness with respect to noise. Through an extensive in silico study of models of two known biological systems, we compare different methodologies and computational approaches to handle noisy data. We look at different perturbation strengths, replicate numbers, and numerical solvers. The proposed analysis brings a deeper understanding of the effects of noisy data on regulatory networks inference, demonstrating that the choice of experimental design and MRA formulation is crucial for a reliable topology estimation.</td>
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| PP4.079 | **Stochastic Dynamics in Sequestration Reduces the Output Variance in Cascades of Phosphorylation/De-Phosphorylation Cycles**  
Debdas Paul, Nicole Radde |
---|---|

The relation between design complexity of signaling network motifs and its robustness against intrinsic noise still remains elusive. In this work, we investigate the role of cascading for coping with intrinsic noise due to stochasticity in molecular reactions. We use stochastic approaches to quantify fluctuations in the terminal kinase of phosphorylation/de-phosphorylation cascade motifs and demonstrate that cascading acts to reduce these fluctuations. We show that this purely stochastic effect can be explained by time-varying sequestration of upstream kinases and that the extent of reduction is crucially dependent on time scales and parameter regimes.

| PP4.080 | **The Muscle Geometry: A Key Factor to High-Amplitude Movement Synthesis with Hill-Type Muscles**  
Maria Hammer, Michael Günther, Daniel F. B. Haeufle, Johannes Walter, Syn Schmitt |
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Muscles play an important role in biomechanics as they exert torques onto the joints. These torques highly depend on the muscle length and geometry as both of them influence the scalar muscle force as well as the muscle line of action. Especially in complex multibody simulations, where reduced descriptions of muscles as massless, visco-elastic, active strands are used, a correct representation of muscle geometry is mandatory. This includes physiological muscle lever arms and pennation angles describing the muscle line of action and the volumetric shape changes of the muscle belly, respectively. To address these issues, we developed a new computational algorithm for modeling the muscle path based on finding the shortest muscle path while the muscle is lead through a small number of ellipses. We furthermore developed a 3D pennation angle model based on analytic geometries, which can be included in any Hill-type muscle model. We applied both methods to a multibody model of the human leg.

| PP4.081 | **Gaining Insight into the Regulation Mechanisms of DLC1**  
Antje Jensch, Katharina Bitschar, Nicole Radde, Monilola Olayioye |
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"Deleted in Liver Cancer 1“ (DLC1) is an important tumor suppressor protein which was found to be downregulated in different tumor types including liver, breast and lungs. The investigation of the regulatory mechanisms of DLC1 is important for the development of therapeutic strategies. In this work we employ a systems biological approach combining experimental data with mathematical modeling based on ordinary differential equations. A Maximum Likelihood based approach is used to infer the model parameters under an appropriate choice of an error model. Resulting model fits are in good agreement with the experimental data. Model plausibility is tested by a parametric bootstrapping approach. Through this study we could reveal the interplay of the key players responsible for the regulation of DLC1.
| PP4.082 | **Digital Human: Towards Realistic HPC Models of the Neuromuscular System**  
Nehzat Emamy, Thomas Ertl, Dominik Göddeke, Thomas Klotz, Aaron Krämer, Michael Krone, Benjamin Maier, Miriam Mehl, Tobias Rau, Oliver Röhrle |
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<td>Within this project, we want to contribute to the grand vision of achieving a virtual physiological human model by developing a realistic model of the neuromuscular system. Due to the high complexity of the system, detailed multiscale models are indispensable. To obtain a close-to-realistic model, we employ HPC to extend the existing computational and modelling frameworks (currently only running on small-scale clusters) to large-scale simulations. Within the open-source OpenCMISS framework, we investigate different modelling, algorithmic and implementational aspects of analysing and optimising the chemo-electromechanical model of skeletal muscle tissues. Moreover, a novel visualisation environment, which is based on the MegaMol environment, has been proposed to visualise the large amounts of simulation data.</td>
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| PP4.083 | **Multiscale Homogenisation-Based Continuum-Mechanical Modelling of Skeletal Muscle Tissue**  
Christian Bleiler, Pedro Ponte Castaneda, Oliver Röhrle |
| | Skeletal muscle tissue – as well as biological tissue in general – shows a wide variation in its mechanical response for different persons or different muscle types of one single person. These distinct mechanical properties are due to variations in the microstructure of the material. For skeletal muscles, especially the arrangement and the stiffness of collagen fibres in the connective tissue define the macroscopic passive stiffness, while the sarcomeres (contractile units) enable an active contractility of the muscles. Phenomenological models lack the ability to take into account such microstructural variations in a natural way and need to be fitted to experimental data, which is, however, not available for every desired muscle type. Thus, this work presents a homogenisation-based multiscale model for skeletal muscle tissue which enables to include microstructural properties directly in a continuum-mechanical macroscale by using well-founded analytical homogenisation techniques. |
| PP4.084 | **Towards an Integrated System for Image Analysis in Brain Tumor Imaging and Quantitative Oncology Based on Inversion Methods**  
Klaudius Scheufele, Andreas Mang, Amir Gholami, George Biros, Miriam Mehl |
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<td><strong>We present a framework for joint image registration and biophysical inversion to analyse MR images of glioblastomas (primary brain tumors). Given (the segmentations) of a normal brain MRI and of a cancer patient MRI, we wish to determine tumor growth parameters and a registration map so that if we ‘grow a tumor’ in the normal segmented image and then register it to the patient segmented image, the registration mismatch is minimal. We call this ‘the coupled problem’ because it two-way couples the biophysical inversion and registration problems. In the image registration step we solve a large-deformation diffeomorphic registration problem whereas in the biophysical inversion step we estimate parameters in a reaction-diffusion tumor growth model. We present a PDE-constrained optimization formulation of the coupled problem and the derivation of a Picard iterative scheme to solve it. We provide numerical results for real brain datasets and show convergence of our coupling algorithm.</strong></td>
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| PP4.085 | **Neuro-Musculo-Skeletal Models as a Tool to Understand Human Motor Control Disorders**  
Katrin Stollenmaier, Christina Pley, Winfried Ilg, Martin Giese, Syn Schmitt, Daniel Häufle |
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<td><strong>How does the human brain control voluntary movement? What happens if these control mechanisms are impaired by a neurological movement disorder? Our goal is to address these questions by combining mathematical models and simulations of the neuro-musculo-skeletal system with recent insights in neuroscience and results from experimental studies. We conduct experiments with healthy subjects and cerebellar ataxia patients performing goal directed upper limb movements. Kinematics are recorded by a motion capture system and together with surface muscle electromyograms. The data is compared with a computer simulation of a neuro-musculo-skeletal model of the human arm with shoulder and elbow joints, actuated by six muscles and controlled by a hybrid equilibrium point controller. Here, the experimental data is the basis for the validation of the model and the development of a better understanding of human movement generation.</strong></td>
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| PP5.086 | **Model-Adaptive Schemes for Reactive, Compressible Flows**  
Jan Giesselmann |
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| **Many physical processes can be described by several different mathematical models which vary in their level of generality and in the amount of detailed information they provide. One example are compressible, reactive flows whose description is significantly simplified once chemical equilibrium is assumed. However, assuming chemical equilibrium is only admissible in certain flow regimes and assuming it in the whole space-time domain of interest may lead to significant errors. This raises the following question: Given a certain error tolerance, in which areas may we replace the complex nonequilibrium model by a simpler one, and in which parts of the domain do we have to use the complex model. The goal of this poster is to describe how this question can be addressed by modeling error estimators, i.e., computable upper bounds for the difference between the solutions of both models.** |
| PP5.087 | **Using a Pore-Network Model to Couple Mass, Momentum and Energy at the Interface Between Free Flow and Porous-Media Flow**  
Kilian Weishaupt, Rainer Helmig |
| **Coupled systems of a porous medium with an adjacent free flow appear in a wide range of industrial and environmental processes. We propose an efficient coupled model comprising three domains: a bulk porous medium (Darcy's or Forchheimer's law) at the bottom, the free-flow domain (Navier-Stokes) on the top and the interface region (dynamic pore-network model) in between. This model can help to provide effective upscaled parameters required for other mechanical modelling approaches.** |
| PP5.088 | **Stochastic Modeling of Flow in Heterogeneous Porous Media**  
Markus Köppel |
| **The modeling of two-phase flow and transport processes in porous media is generally prone to uncertainties in material parameters, source terms or boundary conditions. Based on the capillarity-free fractional flow formulation we quantify such kind of uncertainties by the hybrid stochastic Galerkin method. The intrusive method extends the concept of the polynomial chaos (PC) expansion for a multi-element decomposition of the stochastic space. This results in a deterministic system for the coefficients of the PC expansion of the unknowns. The sequential modeling of the hyperbolic-elliptic system is then discretized with a central-upwind finite volume scheme for the hyperbolic along with a mixed finite element method for the elliptic part. By construction the method is well-suited for massively parallel computations of complex flow problems. Based on a purely hyperbolic problem we assess the accuracy and the convergence of the approach compared to other non-intrusive methods in the field.** |
| PP5.089 | **Advection-Diffusion PDEs with Random Discontinuous Coefficients**  
Andreas Stein, Andrea Barth |
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<td><strong>Advection-diffusion equations arise in various applications, for instance in the modeling of subsurface flows. We consider this type of partial differential equations with random coefficients, which may then account for insufficient measurements or uncertain material procurement. To represent, for example, transitions in heterogeneous media, we include spatial discontinuities in the parameters of the equation. For a given temporal discretization, we solve a second order elliptic problem in each time step where the random coefficient is given by the sum of a Gaussian random field and a (discontinuous) jump part. By combining multilevel Monte Carlo sampling and pathwise finite element methods we are able to estimate moments of the solution to the random partial differential equation. To stabilize the approximation and accelerate convergence, we introduce an adaptive, pathwise triangulation for the finite element approximation which accounts for the varying discontinuities in each sample.</strong></td>
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| PP5.090 | **Modeling Porous Medium Modification Through Induced Calcite Precipitation**  
Johannes Hommel, Robin Gerlach, Alfred Cunningham, Adrienne J. Philipps, Rainer Helmig, Holger Claas |
| **Induced calcite precipitation is an emerging technology to alter properties of porous media. It results in a decrease in porosity and permeability as well as an increase in mechanical strength. For a reliable prediction of these changes, numerical modeling is the method of choice, as the involved processes are strongly coupled. Validated to experimental data, such numerical models are useful tools in the upscaling from laboratory to field-scale applications, which may include subsurface gas storage, soil stabilization, or remediation of a leaky well.** |
| PP5.091 | **An Adaptive Multiphysics Model Coupling Vertical Equilibrium and Full Multidimensions**  
Beatrix Becker, Bo Guo, Karl Bandilla, Michael Celia, Bernd Flemisch, Rainer Helmig |
<p>| <strong>Efficient multiphysics models that can adapt to the varying complexity of physical processes in space and time are desirable for modeling fluid migration in the subsurface. Vertical equilibrium (VE) models are simplified mathematical models that are very fast but rely on the assumption of instant gravity segregation of the two phases. We present a scheme to couple a full multidimensional two-phase flow model to a VE model and develop a criterion that determines subdomains where the VE model is valid during simulation. The VE model is then adaptively applied in those subdomains, while everywhere else in the domain the full multidimensional model is used. We analyze the influence of the threshold parameter for the adaptive algorithm and demonstrate its efficiency and accuracy of the adaptive multiphysics model. We show that the adaptive multiphysics model is much more computationally efficient than the full multidimensional model, while maintaining much of the accuracy.</strong> |</p>
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<tr>
<th>PP5.092</th>
<th>An Adaptive Staggered-Grid Formulation for the Simulation of Porous-Medium Flow Free-Flow Coupling</th>
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<td>Melanie Lipp, Rainer Helmig, Kilian Weishaupt, Martin Schneider</td>
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Flow and transport processes in domains composed of a porous medium and an adjacent free-flow region appear in a wide range of industrial, environmental and medical applications. A turbulent, free, one-phase (gaseous) flow in the atmosphere and a flow in the soil, which might be a two-phase (gaseous and liquid) flow, with different dominating physical processes, are coupled at an interface. Water, energy and gas fluxes are strongly influenced by the flow processes at the soil-atmosphere interface, as well as by the interface topology. In the open-source software DuMuX, the free-flow region uses a staggered grid discretization in order to avoid pressure oscillations. In this grid, velocities are calculated on nodes shifted by half a grid length with respect to the pressure nodes. In order to finely resolve the interface without overly increased computational cost, the present work adds grid adaptivity to the free-flow discretization within DuMuX, making local refinement possible.

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<th>PP5.093</th>
<th>Dynamic Density Functional Theory for Droplet Coalescence</th>
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<td>Rolf Stierle, Joachim Groß</td>
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Thermodynamic analysis of droplets allows insight into nucleation and coalescence phenomena. Using classical Density Functional Theory (DFT), a native thermodynamic approach presents itself to problems including nucleation, coalescence and structure analysis of fluids. DFT is a powerful tool for analysis of interfacial phenomena and prediction of interfacial properties. Helmholtz energy functionals of the PC-SAFT equation of state are used, allowing for the calculation of single droplets without usage of interfacial-specific parameters. Relaxation of the equilibrium assumption yields Dynamic Density Functional Theory (DDFT), which is suitable for the calculation of dynamic density distributions. This contribution presents results from 3-D DDFT calculations of coalescence phenomena.

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<th>PP5.094</th>
<th>Developing and Calibrating a Numerical Model for Microbially Enhanced Coal-Bed Methane (MECBM) Production</th>
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<td>Simon Scholz</td>
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Microbially enhanced coal-bed methane (MECBM) production is an innovative idea to stimulate biogenic coal-bed methane production by providing methanogens and nutrients to the coal and, thus, enhancing the microbial conversion of coal to gas. However, little is known about the environmental conditions favourable to CBM production, or the details of interactions of microbes and nutrients that promote CBM production. A new numerical model is implemented into the Open-Source numerical simulator DuMuX. The relevant processes of MECBM are identified and their interactions are formulated in a conceptual model, including flow and transport of fluids as well as microbiological, chemical, and adsorption/desorption processes. This project is linked to an ongoing experimental DoE-project at Montana State University (MSU) in Bozeman/USA. The project at MSU provides the required inputs to develop a conceptual model and to calibrate and validate it with experimental data.
### PP5.095  Multicomponent Diffusion in a Coupled Free-Flow Porous-Medium System
Katharina Heck, Rainer Helmig

A standard approach to model diffusion in porous media is the assumption of the validity of Fick's Law. That is only true for binary mixtures or low concentrations of the components. When looking e.g. at gas migration of an organic component in soil or fuel cells where higher concentrations of components in liquid and gas can occur, more complex laws need to be employed. In this work we present a model incorporating the Maxwell-Stefan's law of diffusion for the component transport in the free-flow and the porous medium unsaturated flow. Consistent coupling conditions for the two regimes are presented and the influence of different concentrations of components in a multiphase mixture are studied. One main example which is presented is evaporation together with gas migration in the porous medium and across the porous-medium free-flow interface.

### PP5.096  Experimental and Numerical Investigation of Sublimation Processes of Supercooled Ice
Martin Reitzle, Stefano Ruberto, Bernhard Weigand

The weather generation in the atmosphere is heavily influenced by the temperature and pressure distributions which are in turn affected by phase change processes on the small scales. These phase change processes – solidification, sublimation or evaporation – take place at temperatures well below the freezing point of water. We will present our recent progresses in experimental and numerical work focusing on sublimation processes at these conditions. To this end, an experimental facility is used where single droplets are optically levitated. The temperature and relative humidity can be varied. Using a shadowgraphy technique, the evolution of the diameter of the ice particle over time is tracked. Furthermore, a novel numerical technique is presented which allows to simulate the sublimation process within a Volume-of-Fluid framework. One particular challenge is the description of the local thermodynamic equilibrium at the phase boundary. The results are compared to experimental data.

### PP5.097  Implementation of Structured Surfaces in Free Surface 3D (FS3D)
Corine Kieffer-Roth, Martina Baggio, Bernhard Weigand

The aim of the present work is the implementation of structured surfaces in the DNS, Volume of Fluid multi-phase code FS3D. Since FS3D is based on Cartesian grids, a method to represent embedded solid boundaries on Cartesian meshes is required. In the approach proposed here, the boundary is described by the value of its volume fraction $f_b$ in each computational cell. In the cells where $0 < f_b < 1$, the boundary surface is approximated with a plane (PLIC method). So far, the work has focused on the advection of momentum and of the fluid volume fraction $f$. The fluid interface is also reconstructed with the PLIC-scheme. Its orientation in boundary cells is assumed perpendicular to the boundary and its position is determined iteratively. The used operator split advection scheme has been adapted to the presence of the boundary. Calculations for fluid advection on different solid shapes are also shown.
| PP5.098 | **Direct Numerical Simulations of Solid Particles Motion in Newtonian Fluid Flow**  
Nadine Falkner, Holger Steeb |
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<td>Suspensions and their applications can be found in many fields of mechanical, civil and environmental engineering. The rheological behavior of suspensions strongly depends on their concentration. To consider the flow behavior as well as fluid-solid interactions in dilute suspensions, we present Direct Numerical Simulations of a single-phase fluid with embedded solid particles. Simulations are performed using the particle code HOOMD-blue extended for the usage of Smoothed Particle Hydrodynamics (SPH). When it comes to large displacements or when fully resolved hydrodynamic forces are needed, SPH as a meshfree Lagrangian method presents huge advantages compared to often used DEM approaches. A simplified Hertz-Mindlin contact model was implemented to describe solid particle interactions. Our study shows the evolution of shear flow dependent on the number of suspended particles where the flow is mainly dominated by hydrodynamical forces up to aggregate network forces.</td>
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| PP5.099 | **Mixed-Dimension Models for Root-Soil Interaction and Root Growth**  
Timo Koch, Katharina Heck, Holger Class, Rainer Helmig |
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<td>We present a consistent model concept and a flexible software framework for modeling fluidmechanical processes in the vadose zone including root systems. Such processes include contaminant transport, tracer experiments, root water uptake, root growth, evaporation and transpiration. The root system architectures are represented discretely using reduced-dimensional models. There are embedded in a three-dimensional environment and exchange mass and energy with the surrounding soil. The presented numerical scheme is locally mass-conservative, even in the context of mixed-dimensional coupling and root system growth. We investigate evaporation from soil and plant transpiration as competing processes driving the soil-atmosphere water transfer.</td>
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| PP5.100 | **Towards a Scalar Flux Model Based on Tensor Representation Theory and Machine Learning**  
Corrado Sotgiu, Bernhard Weigand |
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<td>The performance of a gas turbine is greatly affected by the maximum cycle temperature reached by the hot gas, which exceeds the melting point of the turbine blade material. To further improve blade cooling, the need for accurate heat transfer predictions by means of CFD is strongly increasing. While great advancements have been made in the development of turbulence models for the Reynolds stress tensor, the heat flux vector modeling relies in most cases on the gradient-diffusion hypothesis. This approach provides an isotropic thermal diffusivity, which is known to be inaccurate. Tensor representation theory can be used to derive an anisotropic thermal diffusivity with an algebraic formulation, but the determination of the model coefficients is still an unresolved problem. Here, a novel procedure, based on machine learning, is proposed. Large quantities of DNS data are used to train neural networks and provide an accurate fitting of the model coefficients in different flow regions.</td>
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| PP5.101 | **High-Dimensional Surrogates with B-Splines for UQ and Multi-Scale Problems**  
Michael Rehme, Dirk Pflüger |
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<td>Sparse grids and the sparse grid combination technique are well-established methods to deal with high-dimensional problems. Classic approaches use hat functions or global polynomials which can lead to non-differentiable or possibly instable interpolants. We propose using B-splines as basis functions to overcome both problems and apply this ansatz to two applications. The first one deals with uncertainty quantification where we introduce a not-a-knot B-spline basis for anisotropic full grids to cope with inaccuracies at the boundary of the stochastic domain and reduce the total costs using adaptive refinement. Our second application is a multi-scale model reduction in process engineering. We use characteristic maps to integrate models on a micro scale into macro scale models allowing e.g. the simulation of the flow through a catalyst bed.</td>
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| PP5.102 | **Model-Based Visual Analysis of Large Spatiotemporal Data**  
Gleb Tkachev, Steffen Frey, Thomas Ertl |
| Simulations generate large data that can also have multi-variate and multi-run aspects. This makes classic specialized visualization techniques difficult to apply directly. We propose a more general approach, utilizing machine learning to gain insights from the data. Specifically, we train a model to act as a surrogate model for a dataset, predicting data values based on the values that occurred in the past. We then analyze both the model parameters as well as the prediction. For instance, we find regions of space and time where the prediction deviates from the actual data. The behaviour there is complex and unpredictable, such that the model failed to capture it during training. This information can be used to highlight important events during direct visualization, but also to sparsify the data before aggregation. We perform integrated rendering of the selected regions to construct a succinct overview of the data. We evaluate our method across different models and application domains. |
| PP5.103 | **Direct Numerical Simulations of Evaporating Droplets under Various Conditions**  
Karin Schlottke, Jonathan Reutzsch, Bernhard Weigand |
| The numerical simulation of multiphase flows is important to describe many processes in nature and engineering. In a lot of these applications, it is not only the coexistence of different phases which is of interest, but it is rather the heat and mass transfer including phase change between them around which the focus of research is centered. The presented investigation covers three-dimensional numerical simulations of liquid-gas phase change using the direct numerical simulation code FS3D. This in-house code solves the incompressible Navier-Stokes equations and uses the Volume-of-Fluid (VOF) method in order to account for multiple phases. The convective transport is performed based on the piecewise linear interface calculation (PLIC) of the surface. Various simulations of evaporation processes, from supercooled water droplets in clouds to fuel droplets inside a combustion chamber to droplets near the critical point, are presented in order to show the wide applicability of the code. |
| PP5.104 | **A Posteriori Analysis for the Euler-Korteweg Model**  
Dimitrios Zacharenakis, Jan Giesselmann |
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<td>Recently, Giesselmann and Pryer (2016) studied a discontinuous Galerkin (DG) scheme in a multiphase problem of elastodynamics. They derived a posteriori error estimates for the difference of the numerical and the exact solution. Based on this, our goal is to provide a posteriori analysis of a DG scheme for the approximation of the one-dimensional isothermal Euler-Korteweg (EK) system. We discretize EK using a local DG (LDG) formulation. A possible approach to bound the difference between the exact and the numerical solution would be to use the relative entropy technique. However, the energy density has a multi-well shape. Thus, a fundamental component of our analysis is the reduced relative entropy stability framework, and to be able to apply it we introduce sufficiently regular intermediate functions called reconstructions. Since this involves elliptic reconstructions, part of the a posteriori error estimator resembles the estimator given by Karakashian and Pascal (2006).</td>
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| PP5.105 | **Radial Basis Function Mapping for Multi-Physics Applications**  
Florian Lindner, Amin Totounferoush, Miriam Mehl |
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<td>RBFs are an accurate interpolation method for black-box surface coupled multi-physics simulations with non-matching meshes where we have scattered surface data. Non-homogeneous data distributions (in high-order or adaptive discretizations) and the global support of radial basis functions are challenges in terms of accuracy, efficiency, and scalability. We present tailored RBF methods for large, distributed multi-physics scenarios. The interpolation is augmented by a global low-order polynomial and presents a way to separately compute the polynomial. This, along with cut-off basis functions, which maintain a sparse structure of the interpolation system and a tolerable condition. We further improve accuracy and condition with a rescaling approach for the interpolant and the basis functions. All methods are implemented in the open-source library preCICE. It provides data-mapping, accelerated fixed-point iteration schemes for the overall coupled system, and inter-code communication</td>
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| PP5.106 | **Transfer and Intercomparison of Data-Driven Uncertainty Quantification Methods for Two-Phase Flow in Carbon Dioxide Storage**  
Markus Koeppel, Fabian Franzelin, Ilja Kroeker, Gabriele Santin, Dominik Wittwar, Andrea Barth, Dirk Pflüger, Wolfgang Nowak, Haasdonk Bernard, Christian Rohde, Sergey Oladyshkin |
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<td>There are various promising approaches recently available in the literature that have a great potential for the quantification of uncertainty arising within the modeling of flow and transport in carbon dioxide storage. In this work, we transfer and discuss several recent versions of efficient techniques established in different research areas onto the data-driven uncertainty quantification analysis for carbon dioxide storage. We consider the following recent versions of intrusive and non-intrusive model reduction techniques: hybrid stochastic Galerkin method as well as arbitrary polynomial chaos, spatially adaptive sparse grids and kernel based greedy interpolation techniques. We demonstrate the performance of each approach assessing expectation and standard deviation of the carbon dioxide saturation against a reference solution. Assessing</td>
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convergence of the introduced methods, we also present an intercomparison in terms of precisions and corresponding computational efforts.

**PP5.107**

**Visual Analysis of Interface Deformation in Multiphase Flow**  
Alexander Straub, Sebastian Boblest, Grzegorz Karch, Thomas Ertl

In multiphase flow, the interplay of fluid dynamic forces and surface tension leads to the generation of intricate interface formation and potential phase disintegration. The analysis of these kinematics can help in the investigation of interface instability and identification of potential breakups. We present an approach to compute interface stretching and bending based on metric and shape tensors, respectively. For the visual analysis of interface stretching, we employ the eigenpairs of the metric tensor for visualization on the reconstructed interface. We visually analyze interface bending with a technique that locally captures the interface curvature change in terms of a shape tensor. To demonstrate the significance of our method, we apply it to the simulation of a droplet-film interaction resulting in a splash. We compare the results of the simulation with and without consideration of the Marangoni forces to analyze their influence on the splash dynamic.

**PP5.108**

**The Influence of Functional Properties of Plant Tissues on their Frost Resistance**  
Lukas Eurich, Shahla Shahmoradi, Arndt Wagner, Wolfgang Ehlers

Plant tissues have developed several strategies to cope with multiple cycles of freezing and thawing events without being damaged. Understanding the involved strategies and mechanisms of plants upon freezing is of high interest, as they could potentially be used for the development of bio-inspired construction materials, conventional construction materials are frequently damaged under repeated cycles of freezing and thawing. Since the involved thermo-hygro-mechanical processes in plant tissues are strongly coupled, a modelling approach based on the Theory of Porous Media (TPM) is used. An application of this approach allows for a thermodynamically consistent description of key mechanisms with regard to frost resistance of plant tissues, such as the cell dehydration, the water-management capability and the freezing of pore water at species-specific and tissue-specific locations. Selected numerical examples illustrate these effects.

**PP5.109**

**Simulating a Thermochemical Heat Storage Reactor**  
Gabriele Seitz, Holger Claas, Rainer Helmig

Thermochemical heat storage has a large potential due to its high storage densities. In the range of high to medium temperature heat storage the system Calcium oxide–Calcium hydroxide is of special interest, as it reacts at manageable temperatures (300–500 °C), is environmentally friendly and financially attractive. In order to develop a technical application, the processes of the chemical reaction have to be investigated: The granular material undergoes a volume change so that its porosity and permeability and thus the flow processes of the water vapor are changed. Furthermore, the reaction kinetics and the cycling stability have to be examined. To understand the processes and estimate their relevance on the different scales, a 1D numerical model is built in the open-
source simulator DuMuX. The constitutive relations of the complex system are depicted in a multiphase system. Changes in the structural properties such as porosity and permeability are considered.

**PP5.110**

**A Discrete Fracture Model for Complex Flow Processes in Fractured Porous Media**  
Dennis Gläser, Rainer Helmig, Bernd Flemisch

We present a discrete fracture model on the basis of a cell-centered finite volume scheme with multi-point flux approximation, where the fractures are modeled as (n-1)-dimensional entities embedded in an n-dimensional domain. The n-dimensional grid is constrained such that its element facets coincide with the fracture geometries. While this imposes a restriction on the gridding, it comes with the benefit that the model can naturally handle both low and highly permeable fractures. In this work we first investigate the performance of the scheme for increasing physical complexity on simple geometries and in a subsequent step the scheme is applied to more realistic and complex geometries.

**PP5.111**

**Probing the Dynamics of Self-Electrophoretic Swimmers using Lattice Boltzmann**  
Michael Kuron, Georg Rempfer, Joost Graaf, Christian Holm

Many simulational studies are available of the rich transient and collective behavior in catalytically driven colloids, or microswimmers. However, virtually none consider both the hydrodynamic and phoretic fields and most do not take into account even one of them. We introduce a continuum model based on the Lattice-Boltzmann (LB) method that incorporates both effects and is capable of simulating the dynamic behavior of many swimmers. Our swimmers propel via experimentally relevant self-electrophoretic mechanisms with bulk reactions. In order to achieve this goal, we supplement LB with a lattice-based electrokinetics solver, add moving boundary conditions, and model the surface reactions as flux boundary conditions.

**PP5.112**

**A Multi-Phase Model for Chemical Induced Phase Transition**  
Malte Sauerwein, Holger Steeb

In mechanized tunnelling the gap between the tunnel structure and the surrounding soil needs to be filled with an adequate grouting mortar to ensure a rapid and safe bedding of the segment rings in order to minimize settlements above the tunnel lining. After mounting the segment rings, a rapid solidification of the mortar, usually by consolidation, should prevent possible surface displacements. The effective stress evolution of the mortar depends therefore strongly on the permeability of the surrounding soil. In order to overcome this restriction, the use of superabsorbent polymers (SAP) as additive to the grouting mortar has been investigated. When SAPs come in contact with an aqueous solution, they are able to absorb high amounts of the solution under forming a hydrogel. This multi-phase functional material is modeled within the framework of the Theory of Porous Media, while constitutive modeling regarding the phase transition is formulated in a thermodynamic-consistent manner.
| PP5.113 | **On the Influence of Numerical Model Parameters within a Simulation of Two-Phase Flow in a Compressor Cascade**  
Adrian Seck, Bernhard Weigand |
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The usage of regenerative energy results in stronger power fluctuations which have to be balanced by conventional power plants. For stationary gas turbines, the injection of water into the compressor inlet, also called high-fogging, can rapidly increase the power output. This is a result of the evaporative cooling within the compressor. However, a significant part of the water interacts with the compressor blades where various phenomena like splashing, development of a wall film and disintegration of liquid ligaments occur. As experimental investigations at real flow conditions are extremely difficult, numerical modeling comes into play. A one-way coupled numerical model using an Euler-Lagrange approach has been developed to simulate the small scale processes of the droplets. The current study investigates the influence of different model parameters on the wall film solution. Especially the significance of the number of trajectories is investigated and will be pointed out in detail. |

| PP5.114 | **Adaptive Discontinuous Galerkin Methods for flow in porous media**  
Birane Kane |
---|---|
We present an adaptive Discontinuous Galerkin discretization for the solution of porous media flow problems. We implement and evaluate numerically interior penalty DG methods for incompressible, immiscible, two-phase flow. We consider a strongly heterogeneous porous medium and discontinuous capillary pressure functions. We write the system in terms of a phase-pressure/phasesaturation formulation. First and second order Adam-Moulton time discretization are combined with various interior penalty DG discretizations in space. This implicit space time discretization leads to a fully coupled nonlinear system requiring to build a Jacobian matrix at each time step for the Newton method. The adaptive approach implemented allows for refinement/coarsening in both the element size, the polynomial degree and the time step size. This strategy allows to refine the mesh when the solution is estimated to be rough and increase the local polynomial degree when the solution is estimated to be smooth. |

| PP5.115 | **Interface Reconstruction in the Vicinity of Three Phase Contact Lines for Static Contact Angles**  
Johanna Potyka, Corine Kieffer-Roth, Kathrin Schulte, Bernhard Weigand |
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An algorithm for reconstructing PLIC surfaces in the vicinity of three phase contact lines formed by solid, fluid and gas was developed for three phase problems with a volume of fluid method. The basic ideas are taken from Pathak et al. [DOI: 10.1016/j.jcp.2015.11.062] and are adapted and extended for the needs of the ITLR inhouse DNS-code FS3D for incompressible multiphase flow problems. The interfaces in three phase cells are reconstructed by a given contact angle which is set between the normal vectors of the solid and fluid phase. The second angle of the PLIC surface in a cell is found by minimising the error in a stencil around the contact line cell of the volume enclosed by the surface compared to the computed volume. This work is a basis for extending
the interface reconstruction to dynamic contact angle problems and contact lines formed by two immiscible fluids.

**PP5.116**

**Nonlinear Finite-Volume Schemes for Complex Flow Processes and Challenging Grids**  
Martin Schneider, Bernd Flemisch, Rainer Helmig

The numerical simulation of subsurface processes requires efficient and robust methods due to the large scales and the complex geometries involved. To resolve such complex geometries, cornerpoint grids are the industry standard to spatially discretize geological formations. Such grids include non-planar, non-matching and degenerate faces. The standard scheme used in industrial codes is the cell-centered finite-volume scheme with two-point flux (TPFA) approximation, an efficient scheme that produces unconditionally monotone solutions. However, large errors in face fluxes are introduced on unstructured grids. The authors present a nonlinear finite-volume scheme applicable to corner-point grids, which maintains the monotonicity property, but has superior qualities with respect to face-flux accuracy. The scheme is compared to linear ones for complex flow simulations in realistic geological formations.

**PP5.117**

**B-Splines on Sparse Grids: Algorithms and Application to Real-World Optimization**  
Julian Valentin, Dirk Pflüger

In simulation technology, models often depend on a number of unknown parameters, for example coefficients in partial differential equations. The inverse problem is to determine the optimal parameters such that the simulation matches reality best. As the models become more complex, the number of parameters increases and the solution of the corresponding optimization problem becomes hard, especially if the simulation is time-consuming. We replace the costly simulation with a surrogate based on sparse grid interpolation with B-splines as new basis functions. This enables higher convergence rates while coping with the curse of dimensionality. The project is split in two interconnected parts: First, we study algorithmic implications of the new basis. Second, we investigate three real-world applications of the new method in collaborations: a biomechanical application (together with O. Röhrle/SimTech), an application in topology optimization, and an application from financial mathematics.

**PP5.118**

**Large Scale SPH Simulation of Single Phase Flow Through Porous Media: Scalability Study**  
Maria Osorno, Malte Schirwon, Nadine Falkner, Holger Steeb, Dominik Göddeke

The numerical study of fluid flow through porous media is highly relevant in several fields, such as dioxide sequestration, geothermal energy generation and groundwater contamination remediation. To simulate the fluid single-phase flow at pore-scale, we employ a quasi-incompressible Smoothed Particle Hydrodynamics (SPH) method. SPH is a meshless Lagrangian method, highly suitable for modeling complex geometries and flow at high Reynolds numbers. However, SPH requires high computational resources, especially for the
simulation of large domains. To overcome this difficulties, we implemented the SPH method in the highly optimized software HOOMD-blue. This software was designed for general-purpose particle interaction simulations and is CPU and GPU parallelized. We study the performance of our implementation employing the CPU parallelization, and carried on a scalability study in the HLRS super computer Hazel Hen.

### PP5.119
**Hydro-Mechanical Coupling using Hybrid Dimensional Elements and Non-Conformal Meshes**  
Patrick Schmidt, Holger Steeb

Subsurface flow in porous and fractured media gives insights into fluid underground storage and underground matter and heat transport. Traditionally diffusion based models precisely describe subsurface flow. Nevertheless, when hydro-mechanical effects such as inverse water level fluctuations (Noordbergum effect) are of interest diffusion based models lack to reproduce the physical behaviour. Theoretically Direct Numerical Simulations or coarse-grained continuum approaches can reproduce these phenomena. However, methods with an explicit representation of the fracture domain fail for fractures with high aspect ratios (length vs aperture > 1000). Hence this work uses a hybrid dimensional model for the fracture domain which reduces the model dimension by one. The fracture domain is coupled to the bulk material in an iterative scheme to find the equilibrium state for every time step. To improve the efficiency, the discretization of both domains are non-conformal.

### PP5.120
**Greedy Function Approximation with Matrix-Valued Kernels**  
Dominik Wittwar, Bernhard Haasdonk

We are interested in approximating vector-valued functions on a domain $\Omega$. We consider reproducing kernel Hilbert spaces of $\mathbb{R}^m$-valued functions which admit a unique reproducing kernel $k$ which is matrix-valued. These spaces seem promising, when modelling correlations between the target function components. The approximation $s_f$ for a function $f$ takes the form

$$s_f(x) := \sum_{i=1}^{n} k(x, x_i) \alpha_i \text{with centers } x_i \in \mathbb{R}^m.$$  

To guarantee a fast evaluation the number of centers $n$ is desired to be small. We thus present 3 different algorithms by which a suitable set of centers is chosen: First, the $P$-Greedy which requires no function evaluations. Second and third, the $f$-Greedy and $f/P$-Greedy which require function evaluations but produce centers tailored to the target function. The efficiency of the approaches is investigated on some data from artificial models and real engineering applications.
| PP5.121 | **Numerical Treatment of Boundary Layers for High-Order DG Schemes**  
Serena Vangelatos, Claus-Dieter Munz |
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<td><strong>Large Eddy Simulations (LES) of high Reynolds number flows becomes exceedingly expensive, if boundary layers have to be resolved. Beside separation phenomena or interaction of the boundary layer with the outer flow the accurate resolution of the turbulent structures within the layer is not needed and can be modeled. Several techniques for wall-modeled LES exist to model the nearwall turbulence and momentum transfer. The novel Extended Discontinuous Galerkin scheme (XDG) exploits a priori properties of the expected form of the solution for resolving steep gradients within the layer. The main idea of this approach is to enrich the polynomial solution space of the Discontinuous Galerkin Spectral Element Method by an appropriate function, which is adopted to the flow features and is non-polynomial. Applied to turbulent boundary layers, we can make use of the universal properties of the mean velocity distribution to resolve the velocity gradients in the near-wall region with coarse meshes.</strong></td>
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| PP5.122 | **Balanced-Force Numerical Framework for Immiscible Two-Phase Flow at the Onset of Instability**  
Hrishikesh Joshi, Duncan van der Heul, Ruud Henkes |
| **The Interface Capturing method (ICM) (P. Queutey and M. Vissoneau, An interface capturing method for free-surface hydrodynamic flows, Computer and Fluids (2007)) for immiscible multiphase flows employs a collocated grid and achieves a discrete force balance for the case when the interface coincides with the faces of the control volumes. In the present research an extension of ICM is formulated, applicable for an interface that neither has to coincide nor be aligned with the faces of the control volumes. The approach consists of the reconstruction of the flow variables at the interface based on the interface jump conditions. Furthermore, the construction of the operators in the discrete system to achieve a discrete force balance is delineated. The resulting framework avoids the occurrence of spurious velocities and produces physically consistent numerical solutions. Results are shown for steady and unsteady test cases and compared with numerical results obtained with OpenFOAM.** |
| PP5.123 | **Dissipative Particle Dynamics Study of Assembly and Co-Assembly of Poly(N-Isopropylacrylamide) with Carboxyl and Docecyl Terminal Groups in Aqueous Solutions**  
Karel Šindelka, Miroslav Štěpánek, Karel Procházka, Zuzana Limpouchová |
| **Thermoresponsive polymer PNIPAm has interesting applications as, for example, a component of drug delivery systems [1]. Addition of various terminal groups further enriches its multi-responsivity, e.g. PNIPAm with dodecyl and carboxyl terminal groups (HOOC-PNIPAm-C12) forms in aqueous solutions micelles responsive also to pH or ionic strength [1]. We studied self-assembly of HOOC-PNIPAm-C12 and its co-assembly with ionic surfactants in aqueous solution using dissipative particle dynamics with explicit electrostatics [3]. We parameterized our model according to experimental results [3] and performed an extensive parametric study to elucidate experimental data.** |
A Linear Domain Decomposition Method for Two-Phase Flow in Porous Media

David Seus, Christian Rohde, Florian Radu, Iuliu Sorin Pop, Koondaibha Mitra

Soil remediation, CO2 storage and harvesting of geothermal energy are notable examples of multiphase flow processes through porous media. Modelling these processes leads to coupled nonlinear partial differential equations that change type and involve largely varying physical properties of the soil, like porosity and permeability and make the design of robust discretisation methods a nontrivial task. We combine a globally convergent L-scheme with a non-overlapping domain decomposition of the two-phase flow equations making use of a linearised Robin type interface conditions to decouple both problems and obtain a globally convergent scheme which is robust, compares well even against a Newton iteration, and allows to account for very heterogeneous soil properties. We present an analytical convergence result and discuss numerical experiments. This is joint work with Koondanibha Mitra (TU/e), Florin Radu (UIB), Sorin Pop (Hasselt University) and Christian Rohde (Univ. of Stuttgart).

On Probabilistic Transformations and Optimal Sampling Rules for Surrogate Based Inverse Uncertainty Quantification Problems

Fabian Franzelin, Dirk Pflüger

Surrogate based methods such as the polynomial chaos expansion (PCE) or sparse grids (SG) are commonly used in the context uncertainty quantification (UQ). They rely on building a surrogate model of a computationally demanding model that depends on a set of random input parameters. However, the efficiency the surrogate models decrease significantly if the model inputs are stochastically dependent and if their stochastic properties are described by data. This poses limits to solve Bayesian inverse problems where usually non-i.i.d. data arises. This poster will discuss probabilistic transformations that decorrelate random variables for improving the efficiency of Bayesian inverse problems. We will present numerical studies that demonstrate the effectiveness of these transformations and present some alternatives such as weighted L2-Leja sequences in combination with PCE, and the integrated adaptive SG approach. We show recent results on data-driven UQ for a CO2 storage problem.
The characterisation of porous media can be understood from a multi scale approach. The transport, mechanical, electrical and magnetic effective properties are directly affected by the processes occurring in the micro scale. X-ray micro computed tomography is able to find the local value of the absorption coefficient of the scanned material, which can be translated into the material density. From this density scalar field, it is possible to reconstruct the volume’s internal geometry, which can be used as an input for numerical simulations. In situ experiments in XRCT, captures simultaneously the internal processes in the material, and the internal structure information for simulations. We present a complete workflow comprising the sample preparation, experimental design, XRμCT device design, image post processing and some examples of numerical simulations from the acquired geometries. Additionally, we show a comparison from the simulations and the in situ experimental results.
| PP6.127 | **Towards Comparable Visual Representations for Biomolecules**  
|         | Karsten Schatz, Michael Krone, Thomas Ertl |
|         | The visual inspection of biomolecular data sets is a crucial step for their analysis. Often, abstracted visualizations are helpful tools to gain insight into the properties of said biomolecules. While the known and established visualization methods work well for single molecules, the comparison of multiple entities still might be difficult. For example, the complex geometry produced by molecular surface methods effectively prevents a direct comparison of these surfaces, especially when the viewer is not able to interact with the visualization. To overcome these issues, we present methods designed to enable the user to easily compare the visual representations of biomolecules qualitatively as well as quantitatively. This includes, among others, a mapping of molecular surfaces to a plane, which results in a map-like representation of the surface features. |
| PP6.128 | **Utilizing Networked Mobile Devices for Scientific Simulations**  
|         | Christoph Dibak |
|         | Emerging augmented reality devices enable novel, interactive simulations. Simulation results no longer need to be viewed on a computer screen but can be overlayed over real-world objects like complex machinery. This supports engineers in making better decisions in the field. However, having interactive simulation results available on mobile devices like augmented reality headsets is challenging since such battery-powered mobile devices are restricted in computational power, have limited energy resources, and are subjected to intermittent connectivity. Additionally, the execution of simulations is hard to distribute between heterogeneous devices. In our research, we developed different methods that can be used for the distribution of the computation between mobile device and remote server. Our approaches significantly improve latency, dynamically adapt quality, and provide simulation results even in harsh environments. |
| PP7.129 | **Setting the Frame for Simulating Complex Social Scenarios**  
Tom Poljansek |
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| | Within the next decades, social simulation will become increasingly influential and important for a number of diverse areas. Political decision makers, entrepreneurs, as well as advertisers are, among others, highly interested in the ability to predict and control human behavior within different interaction scenarios. However, as renowned social simulators like Bruce Edmonds, Emma Norling and Yoshihisa Kashima have emphasized, the actor-models mostly used within current social simulations are still too simple to account for complex social scenarios involving human agents and their real conduct. Based on the results of our research on human agency and interaction within shared worlds I will outline boundary conditions for the simulation of different types of interaction scenarios, thus setting the criterial frame to further improve the simulation of complex social scenarios in the near future. |

| PP7.130 | **An Energy Storage Simulation Model and its Impact on Decision Making**  
Maximilian Happach, Meike Tilebein |
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| | By signing the Kyoto protocol and the Paris Agreement, the German government committed to a mitigation of greenhouse gas emissions of 80% by 2050 compared to the level of 1990. In order to ratify the international treaties, the German government imposed several measures, including the renewable energy sources act and the climate action plan. Both point out the importance of renewable energy technologies especially those based on wind and solar as a key for reaching the target. The diffusion of these renewable energy technologies has initiated an energy transition that has been leading to a shift in generation technologies. This shift replaces a stable, predictable and thus secure but greenhouse gas emitting conventional power generation by a clean, sustainable but less predictable and volatile generation. This poster looks at the current situation and presents a simulation model to analyze the role of energy storage as stabilization of the volatile electricity generation. |
Social Programme
Welcome Reception

- Monday, 26 March 2018
- 6:30 pm – 9:00 pm
- Universität Stuttgart, Pfaffenwaldring 47, 70569 Stuttgart

At the opening day of the SimTech 2018 conference a welcome reception will take place at the foyer of the building Pfaffenwaldring 47. SimTech invites all participants to come together with snacks, drinks and music. In a pleasant atmosphere, our guests get the perfect opportunity to network and to get to know each other.
Conference Dinner

📅 Tuesday, 27 March 2018
⏰ 8:00 pm
📍 Mercedes-Benz Museum

A festive conference dinner will be held on 27 March 2018 in the architecturally unique Mercedes-Benz Museum in Stuttgart.

The Museum celebrates the automobile invented by Carl Benz in 1886: It relates its history and tells its stories, bringing both alive by placing them in the context of technology, day-to-day life, social history and popular culture. More than 160 vehicles of all types are the main protagonists. They range from some of the oldest automobiles ever built to legendary racing cars and futuristic research vehicles. Together with other exhibits, they form the centerpiece of the permanent exhibition covering a total of 16,500 square meters in twelve rooms.

After the Keynote Lecture by Jan Hesthaven, a shuttle bus will depart at 6:00 pm from the university, bringing you straight to the museum.

Here, you can explore the museum on your own and visit the famous exhibition. Audio guides will introduce you to the exciting history and the automobile manufacturer.
The tour is followed by a dinner which is accompanied by a dinner speech by Dr.-Ing. Sabine Lutz, Vice President Group Research and Sustainability, Daimler AG, Stuttgart.

Dr. Sabine Lutz has been working for Daimler since 1996. Following various different positions in production, MBC Assembly Planning and Audit Procurement & Supply, in 2004 she took on the management of the Product Planning Truck Powertrain department. In 2012 she transferred to Corporate Audit in the CEO’s central division, where she was assigned Head of Audit Automotive. Since early 2014 she has managed the Product Platform Transmissions & Axles Truck Powertrain, where she has pushed forward the unit’s global footprint, the introduction of global module teams and continued the optimization of product costs. In August 2015, she took on the Management of International Procurement Services and, besides of procurement and purchasing, implemented a new spirit and joint collaboration between purchasing and technical/functional departments. In January this year, she started working as head of Group Research and Sustainability within the Research and Development Ressort of Daimler.

The event finishes at around 11:00 pm, when a bus shuttle brings you back to the university via various stops in the city centre of Stuttgart.
About SimTech
SimTech is an interdisciplinary research cluster in the field of simulation technology. More than 200 scientists from almost all faculties of the University of Stuttgart are working on a common goal: They want to pave the way towards an integrative simulation science. By doing so, the Cluster of Excellence “Simulation Technology” has significantly advanced both breadth and depth of simulation science since 2007.

Our mission is to advance simulation technology from isolated numerical approaches to an integrative systems science, grounded in fundamental research, ready for industrial applications and reflected in pure political and social frameworks. This differs substantially from traditional approaches.

In order to achieve these goals, it was and is our aim to foster simulation technologies through interdisciplinary research and to generate and maintain scientific and structural innovations within the entire university.
Stuttgart and Tourist Information
Stuttgart Region – Live your inspiration

**Tradition and innovation** go hand in hand in Stuttgart and its surrounding region to create an exciting interplay. As a region known for its strong economy and scientific prowess, with a wide range of cultural, leisure and recreational activities on offer, Stuttgart is an ideal and inspirational event location.

**This vibrant metropolis** in the South of Germany is in season all year round. Stuttgart is varied and inspirational, endearing and unique, tradition-conscious yet full of surprises, relaxing and stimulating. Discover this fascinating city and its surrounding region!

You can look forward to a city with many faces: Stuttgart enthral its visitors with its lively art and culture scene, excels with masterpieces of historical and modern architecture, hosts international sporting events, celebrates merry festivals and colourful markets, offers world-class shopping and a wealth of other unforgettable options. Stuttgart – the holder of the “City with the Highest Quality of Life” award – combines a high-class lifestyle with an atmosphere of welcoming hospitality, and innovative economic strength paired with a high recreational value.

Stages of world renown... with Stuttgart’s State Theatres the region is home to the world’s largest tripartite theatre. Its ballet has enjoyed international acclaim ever since the days of John Cranko and Marcia Haydée, and Stuttgart State Opera has been awarded the coveted title of “Opera House of the Year” many times.
Architectural highlights and outstanding museums together create a unique symbiosis in Stuttgart. Its "culture mile" links the historical Old State Gallery and the Postmodern New State Gallery, the impressive tower of the Academy of Music and the Performing Arts with its collection of organs, and the House of History. The glass cube of the New Museum of Art provides not only interesting insights into the municipal art collections but also wonderful views over the city.

Stuttgart, the cradle of mobility. It was here, in a little workshop, that Wilhelm Maybach and Gottlieb Daimler together invented one of the very first automobiles, and today the city boasts two of the world's most magnificent automobile museums. This is still the site of the main production plants of both Mercedes-Benz and Porsche today, and the people here feel a close bond with the history and tradition of these two global concerns. The spectacular double helix construction of the Mercedes-Benz Museum attracts both automobile and architecture enthusiasts from all corners of the globe, while at the new Porsche Museum the Zuffenhausen sports car specialists display their legendary mobile icons in bold architecture and a sophisticated ambience.

The combination of cosmopolitan flair and green oases makes Stuttgart a city of delightful contrasts. Extensive parks in the heart of town, and idyllic vineyards directly opposite the main railway station provide peace and relaxation. Killesberg Hill Park and the “Wilhelma” – the only zoological and botanical gardens of their kind in the world, invite you to relax and explore. And no fewer than three mineral spas, fed by the most prolific mineral springs in Western Europe, are guaranteed to promote health and wellbeing.

Merry festivals with typical Swabian "gemütlichkeit” in a stylish setting are places for celebration, enjoyment and discovery. There's the lively “Stuttgart Spring Festival”, the elegant “Summer Festival” on warm August evenings, the “Stuttgart Wine Festival” in late summer with its attractively decorated arbours, the Stuttgart Beer Festival or the traditional “Stuttgart Christmas Market” in the heart of town. Once you've experienced the hospitality and the exuberant atmosphere of Stuttgart's festivals and markets, you'll want to return time and again.

Welcome to Stuttgart – the city of automobiles, wine, culture and history.
**Tourist Information**

The tourist information is located next to the main station in the Königstraße, which is the main shopping street in Stuttgart. The address is:

Tourist-Information i-Punkt Stuttgart  
Königstraße 1A  
70173 Stuttgart  
[https://www.stuttgart-tourist.de/en](https://www.stuttgart-tourist.de/en)

From the tourist information a five-minute walk over the Königstraße leads to the Schloßplatz, where the New Castle, the Old Castle and the Art Museum are located. In the surroundings of the Schloßplatz there are various coffee bars.