SWZ Clausthal – Göttingen
Simulationswissenschaftliches Zentrum

SWZ Mini Workshop “Simulation meets AI”

August 15 and 16, 2024
University of Göttingen

This document is available online via
https://tu-c.de/swzworkshop

Schedule

Thursday, 15 August – Morning

From 9:00	**Get together with Coffee** (Physics building, HS 5, University of Göttingen)
9:30 – 9:40	**Welcome note** (Prof. Dr. F. Wörgötter, Chairman of the SWZ board of directors)

9:40 – 10:30	Keynote: **Sustainable Passenger Transport** (Prof. Dr. A. Schöbel)
10:30 – 10:45	**Shortest path planning on grids and graphs** (T. Kulvicius)
10:45 – 11:00	**Track-to-Track Association in a Collective Perception Scenario** (L. M. Wolf)

11:00 – 11:40	**Coffee break** (Foyer)

11:40 – 11:55	**Online Task Planning using Simulated Mental Imagery** (S. Li)
11:55 – 12:10	**Modeling behavior guided by concepts grounded in sensory information** (M. Tamosiunaite)
12:10 – 12:25	**Enhancing NILM Through Innovative Tooling** (M. Bouchur)

12:30 – 14:00	**Lunch** (MPI / Mensa / CaPhy) *(Note: MPI only cash, otherwise EC card payment, not cash!)*

Thursday, 15 August – After noon

14:00 – 14:50	Keynote: **Digital twins to understand complex systems** (Prof. Dr. A. Ecker)
14:50 – 15:05	**Multiscale Computations using Finite Elements** (J.-A. Tröger)
15:05 – 15:20	**Physics-informed deep operator networks for multiscale simulations** (H. Eivazi)

15:20 – 16:00	**Coffee break** (Foyer)

16:00 – 16:15	**Simulation meets AI: Generative Models and Adjoint Method hybrids** (S. Herzog)
16:15 – 16:30	**On modeling and simulation of acoustic cavitation** (R. Mettin)
16:30 – 16:45	**InRecNet – Insect Recognition Model** (C. Seyidbayli)
16:45 – 17:00	**Renewing Active Matter** (P. Zimmer / Y. Pollack)
17:00 – 17:15	**Modeling actin and synapse geometry** (M. Thomas / M. Fauth)

17:20 – 17:30	**Group photo**

From 18:30	**Dinner** (Restaurant "Bullerjahn") *(Note: Self-payer)*

Friday, 16 August – Morning

From 9:00	**Get together with coffee** (Physics building, HS 5, University of Göttingen)

9:15 – 10:30	**SWZ strategy discussion**

10:30 – 10:45	**Coffee break** (Foyer)

10:45 – 11:35	Keynote: **ML supported simulation in deep drilling technology** (Prof. Dr.-Ing. G. Brenner)
11:35 – 11:50	**Digitization in Materials Science** (N. Merkert)
11:50 – 12:05	**Atomistic simulations** (D. Thürmer)
12:05 – 12:20	**Engineered compounds for the recovery of critical elements** (I. Aa. Alhafez)

12:20 – 12:40	**Conclusion and farewell** (Dr. R. Mettin und Prof. Dr. F. Wörgötter)

12:45 – 14:00	**Lunch** (MPI / Mensa / CaPhy) *(Note: MPI only cash, otherwise EC card payment, not cash!)*

Sustainable Passenger Transport

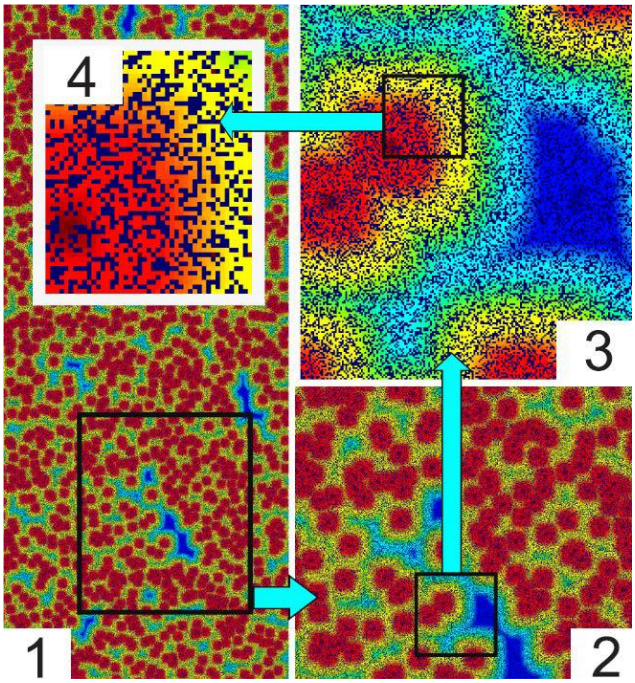
Prof. Dr. A. Schöbel[1]

[1]Fraunhofer Institute for Industrial Mathematics ITWM

Shortest path planning on grids and graphs using networks without and with learning

Tomas Kulvicius[1,2,*], Sebastian Herzog[1], Minija Tamosiunaite[1], and Florentin Wörgöter[1]

[1]Department of Computational Neuroscience, University of Göttingen, 37073 Göttingen, Germany
[2]University Medical Center Göttingen, Child and Adolescent Psychiatry and Psychotherapy, 37075 Göttingen, Germany
*tomas.kulvicius@uni-goettingen.de



Shortest path planning is a fundamental issue in a wide variety of applications, e.g., in computer networks, social networks, trading and finance, multiagent systems, such as games, task, and path planning in robotics, and so on, just to name a few. In the first part of this work [1], we show that it is possible to solve path planning on a grid maze for multiple start- and end-points highly efficiently with a novel configuration of multilayer networks that use only weighted pooling operations, for which no network training is needed. These networks create solutions, which are identical to those from classical algorithms such as breadth-first search (BFS; [2]), Dijkstra's algorithm [3], or TD(0) [4]. Different from competing approaches, very large mazes containing almost one billion nodes with dense obstacle configuration and several thousand importance-weighted path end-points can this way be solved quickly in a single pass on parallel hardware.

In the second part of this work [5], we extend shortest path planning using neural networks to graphs with arbitrary weights. Finding optimal paths in connected graphs requires determining the smallest total cost for traveling along the graph's edges. This problem can be solved by several classical algorithms, where, usually, costs are predefined for all edges. Conventional planning methods can, thus, normally not be used when wanting to change costs in an adaptive way following the requirements of some task. Here, we show that one can define a neural network representation of path-finding problems by transforming cost values into synaptic weights, which allows for online weight adaptation using network learning mechanisms. When starting with an initial activity value of one, activity propagation in this network will lead to solutions, which are identical to those found by the Bellman–Ford algorithm (BF; [6], [7]). The neural network has the same algorithmic complexity as BF, and, in addition, we can show that network learning mechanisms such as Hebbian learning [8] can adapt the weights in the network augmenting the resulting paths according to some task at hand. We demonstrate this by learning to navigate in an environment with obstacles as well as by learning to follow certain sequences of graph nodes. Hence, the here-presented novel algorithm may open up a different regime of applications where path augmentation (by learning) is directly coupled with path finding in a natural way.

References

[1] T. Kulvicius, S. Herzog, M. Tamosiunaite, and F. Wörgöter, “Finding optimal paths using networks without learning – unifying classical approaches”, IEEE Transactions on Neural Networks and Learning Systems, 2021. DOI:10.1109/TNNLS.2021.3089023.
[2] E. F. Moore, “The shortest path through a maze,” in Proc. Int. Symp. Theory Switching, 1959, pp. 285–292.
[3] E. W. Dijkstra, “A note on two problems in connexion with graphs,” Numerische Math., vol. 1, no. 1, pp. 269–271, Dec. 1959.
[4] R. S. Suton, “Learning to predict by the methods of temporal differences,” Mach. Learn., vol. 3, no. 1, pp. 9–44, Aug. 1988.
[5] T. Kulvicius, S. Herzog, M. Tamosiunaite, and F. Wörgöter, “Combining optimal path search with task-dependent learning in a neural network”, IEEE Transactions on Neural Networks and Learning Systems, 2023. DOI:10.1109/TNNLS.2023.3327103.
[6] R. Bellman, “On a routing problem,” Quart. Appl. Math., vol. 16, no. 1, pp. 87–90, 1958.
[7] L. R. Ford, “Network flow theory,” Rand Corp., Santa Monica, CA, USA, Tech. Rep. P-923, 1956.
[8] D. O. Hebb, The organization of behavior. New York, NY, USA: Wiley, 2005.

Acknowledgements

This work was supported in part by the European Community’s H2020 Programme [Future and Emerging Technologies (FET)] under Grant 732266 (Plan4Act) and under Grant 899265 (ADOPD), and in part by the German Science Foundation (DFG) under Grant WO 388/16-1.

Track-to-Track Association in a Collective Perception Scenario

Laura M. Wolf[1], Marcus Baum[1]

[1]Research Group for Data Fusion, Institute of Computer Science, University of Göttingen

We present our recent joint work with Vincent Wolff and Markus Fidler.

A crucial aspect for autonomous driving is the environment perception of vehicles. Equipped with various sensors autonomous vehicles can perceive their surroundings and estimate position and velocity of objects in their vicinity over time.

To further increase the field of view of an autonomous vehicle and the accuracy of the perception they can combine their local perceptions using vehicle-to-everything (V2X) communication. Intelligent vehicles can communicate with each other or with infrastructure modules, such as road side units, and share their local estimates of other objects, the so-called tracks. In the road side unit the local tracks can be combined to a collective perception, which can be useful in areas with many traffic participants, e.g., urban junctions, which can have a lot of occlusions.

As sensor data is noisy, local tracks still have some uncertainty. In the fusion center, i.e., the road side unit, tracks belonging to the same object can be fused together to decrease the uncertainty. Furthermore, the global field of view can be increased by combining tracks from different autonomous vehicles.

Before tracks can be fused, it has to be determined which tracks belong to the same object. The number of possible associations is intractable even for a small number of objects and sensors. We developed a sampling-based association algorithm, that is able to determine associations with a high likelihood in scenarios with a high number of objects and sensors.

As there is no real-world data available for collective perception, we analyzed the association algorithm in a simulated scenario. We used the artery simulator, which combines a traffic simulation with a network simulation for V2X communication. The traffic simulation focuses on a junction and includes vehicles as well as vulnerable road users, such as pedestrians and bicyclists.

We simulate the local environment perception by generating artificial sensor data and then local tracks for all moving objects in the field of view of the autonomous vehicle. The local tracks are sent to the road side unit. Standard track fusion algorithms assume full communication, although this can quickly exceed the capacity of the communication channel. Hence, several strategies to select messages have been considered. Then, the received tracks are associated and fused.

We analyzed the improvement of the fused results over the local perception and how the results of the association are affected, when communication is limited.

Online Task Planning using Simulated Mental Imagery

Shijia Li[1], Minija Tamosiunaite[1], Florentin Wörgötter[1]

1 Third Institute of Physics, University of Göttingen, 37073 Göttingen, Germany
E-mail: worgott@gwdg.de

Task planning in robotics is usually achieved using a symbolically encoded domain description. Humans, on the other hand, perform everyday planning tasks intuitively, using mental imagery of the different planning steps.

Our study shows that a similar approach can be taken also for robots in cases which require only limited execution accuracy. Here we propose a novel sub-symbolic method, which consists of perception, simulated action, success-checking and re-planning performed on 'imagined' images, so called: online Simulated Mental Imagery for Planning (oSiMIP).

Specifically, our method relies on panoptic segmentation, generative object completion and affordance segmentation, all performed by networks, complemented by a search procedure. This produces, by a generative process, a sequence of images leading from the initial state (provided by a 2D top-view) over network-imagined intermediate states (also 2D images) to the final state. Each pair of images in the produced sequence represents the pre-condition and post-conditions for an appropriate action similar to our mental imagery when we imagine the before and after of our own actions.

We create a dataset from real scenes for a packing problem of having to correctly place different objects into different target slots. Then we use two neural networks to provide scene- and affordance-information and we show how to generate a sequence of images that simulates action-outcomes towards a goal. This image sequence, thus, represents the equivalence of a mental, pictorially-imagined plan. When executing these actions, the system compares actual with imagined outcomes and performs online replanning in case of errors. Quantitative results show final success after planning (and – if needed – replanning) in about 94% of the cases.

In conclusion, we propose here a biologically inspired approach for planning, which eliminates the requirement for symbolic pre-structuring, as compared to classical AI approaches and leads to better explainability than end-to-end neural network approaches. This advancement aims to bridge the planning gap between machines and humans, offering a more flexible and adaptable approach to task planning in dynamic everyday scenarios where limited action precision suffices.

Modeling behavior guided by concepts grounded in sensory information

Minija Tamosiunaite[1]

1Third Institute of Physics – Biophysics, University of Göttingen

Current deep-learning-based AI allows integrating a lot of written material humans have created over generations and helps people in abstracting information, learning, making decisions, etc. However, if this type of AI is directly transferable to artificial agents, e.g. robots, and how to do it best is not yet clear. In order to act (and communicate) in real environments, robots have to cover the gap between continuous sensing and action on one side and the pool of symbolic knowledge on the other side. A way for an artificial system to perform a smooth transition from sensor information into concept-like entities is being analyzed by means of modeling in this study.

We take as input simple images and train a small neural network (around a thousand neurons) in environmentally supervised manner to output appropriate action commands in respect to the observed images. Action itself is not modeled in detail but the consequences of the action, resulting in the change of visual input of the model-agent. This way the closed loop is formed. In addition to the above, a second feedback loop is formed using several thousand neurons, where learning is unsupervised. We show that in the second loop concept-like entities, grounded in vision input, emerge. These entities are discreate and connected by relational links to each other, as well as to the sensor layers. The second loop allows to update agent's action commands based on relational information. In this type of processing, phantom images of objects (i.e., not seen by an agent at that specific moment in time) emerge in the visual areas and specifically these agent-imagined images then drive agent's behavior.

The study touches upon the question of smooth signal-to-symbol (and back to signal) transition, visual imagination based on conceptual knowledge and extrapolation beyond the training set. It is shown using simulation that all this allows for an artificial agent to attain behaviors meaningful for the given environment.

Enhancing NILM Through Innovative Tooling for Better Transparency and Performance

Mazen Bouchur[1]

[1]Institute for Informatics, TU Clausthal

Non-Intrusive Load Monitoring (NILM) aids smart energy management by disaggregating a household's total electrical load into appliancespecific consumption without the need for individual appliance sensors.

My previous research developed model compression strategies to enable the efficient deployment of NILM algorithms on edge devices, ensuring their effectiveness in resource-constrained environments. Additionally, I investigated how time-of-day variations in energy consumption can be exploited for model selection, aiming to enhance the accuracy of NILM algorithms through tailored applications.

In response to the growing need for transparency and better adaptability within AI applications, my current research focuses on developing an integrated approach to refine NILM algorithms, aimed at enhancing their applicability and transparency. This effort introduces an innovative tool designed to deepen the understanding of the deep neural networks used in NILM by developers and researchers.

Key functionalities of this tool include:

- **Model Input Inspection and Modification:** Allows manual adjustments or systematic perturbations such as random noise, enabling a deeper understanding of model behavior and its interaction with varied data inputs and under different conditions and scenarios.
- **Empirical Preprocessing Optimisation:** Users can interactively determine optimal preprocessing methods, which may vary significantly across different operating conditions or target appliances, impacting model accuracy significantly.
- **Local Data Insights:** The tool leverages local dataset information to investigate the impact of local conditions like sunrise/sunset times, weekends, or holidays on model behaviour. Features like copy/paste of data samples help simulate and replicate different time patterns to study model responses.
- **Error Analysis:** Users can investigate instances where model performance deviates significantly from expectations—whether errors are too high or too low. A selectable error histogram allows for detailed scrutiny of unique value occurrences and potential measurement errors.
- **Transferability Studies:** Testing model effectiveness across different buildings is streamlined, as models and datasets can be loaded separately, facilitating comparative studies.
- Other Use Cases, like hyperparameters' space exploration and feature map analysis, enable fine-tuning of algorithms to specific contexts and allow for a visual interpretation of how different features influence the model's decisions, thereby offering insights into the neural network's operational dynamics.

These tools and methodologies are designed to not only enhance the transparency and efficacy of NILM algorithms but also to foster a more intuitive understanding among users,

bridging the gap between complex AI technologies and practical energy management applications.

Participating in the workshop and enabling attendees to test the tool firsthand, regardless of their experience level, would provide a valuable opportunity to assess its effectiveness and gather feedback to refine its functionalities and identify areas for future development and potential use cases.

Digital twins to understand complex systems

Prof. Dr. Alexander Ecker[1]

[1]Bernstein Center for Computational Neuroscience Göttingen

Multiscale Computations using finite elements – Computational limitations and machine learning-based remedies

Jendrik-Alexander Tröger[1], Hamidreza Eivazi[2], Stefan Hartmann[1], Stefan Wittek[2], and Andreas Rausch[2]

1Institute of Applied Mechanics, Clausthal University of Technology, 38678 Clausthal-Zellerfeld, Germany, Email address: jendrik-alexander.troeger@tu-clausthal.de,stefan.hartmann@tu-clausthal.de
2Institute for Software and Systems Engineering, Clausthal University of Technology, 38678 Clausthal-Zellerfeld, Germany, Email address: hamidreza.eivazi.kourabbaslou@tu-clausthal.de,stefan.wittek@tu-clausthal.de, Email address: andreas.rausch@tu-clausthal.de

Multiscale computations using finite elements, commonly abbreviated as FE^2, have gained significant interest in recent research due to their ability to account for the heterogeneous microstructure of a material in macroscale computations. In this case, a macrostructure is discretized by means of finite elements, where – at the spatial integration points – the microstructure is resolved by a finite element discretization itself. The wide-scale application of these computations is limited by substantial computational demands, primarily because of the repetitive evaluation of the representative volume elements, which characterize the heterogeneous microstructure. Consequently, the method has not yet become feasible for real applications involving rate-dependent material behavior, uncertainty quantification of the entire simulation, or microstructure optimization for generating new materials.

In this study, first, the algorithmic structure of multiscale finite element computations is described in detail to provide a thorough understanding of the method. Then, we elaborate on integrating a deep neural network as a data-driven surrogate model for the microstructural response. This comprises an innovative strategy for the generation of training data, which leverages knowledge from computational solid mechanics and Sobolev training techniques. The implementation of the surrogate model is thoroughly discussed, highlighting the use of state-of-the-art high-performance computing libraries and just-in-time compilation techniques. Remarkably, this approach leads to a significant computational speed-up of more than 6,000 times compared to a reference FE^2 computation, [1, 2].

References

[1] H. Eivazi, J.-A. Tröger, S. Wittek, S. Hartmann, and A. Rausch. FE2 computations with deep neural networks: algorithmic structure, data generation and implementation. Mathematical and Computational Applications, 28(4), 2023.
[2] J.-A. Tröger, H. Eivazi, S. Hartmann, S. Wittek, and A. Rausch. Efficient integration of deep neural networks in sequential multiscale simulations. PAMM, 23(4):e202300052, 2023.

Physics-informed deep operator networks for multiscale simulations

Hamidreza Eivazi[1], Jendrik-Alexander Tröger[2], Stefan Wittek[1], Stefan Hartmann[2], and Andreas Rausch[1]

[1]Institute for Software and Systems Engineering, Clausthal University of Technology, 38678 Clausthal-Zellerfeld, Germany, Email address: hamidreza.eivazi.kourabbaslou@tu-clausthal.de,stefan.wittek@tu-clausthal.de, Email address: andreas.rausch@tu-clausthal.de
[2]Institute of Applied Mechanics, Clausthal University of Technology, 38678 Clausthal-Zellerfeld, Germany, Email address: jendrik-alexander.troeger@tu-clausthal.de,stefan.hartmann@tu-clausthal.de

Numerical simulations of multiscale problems involving the solution of partial differential equations (PDEs) prove to be computationally prohibitive for tasks such as real-life practical applications, uncertainty quantification, optimization, and control. This limitation has prompted the adoption of *substitutive* surrogate models, wherein micro-scale numerical computations are replaced with data-driven surrogates [1]. While these substitutive surrogates offer a substantial speedup, they tend to be excessively data-hungry and inflexible with respect to various discretizations or different initial and boundary conditions.

In this contribution, we introduce FE-DeepONet, a *complementary*, flexible, and physics-informed learning-based PDE surrogate designed for predicting micro-scale physics through the utilization of operator networks. We showcase the applicability of our framework for multiscale finite element (FE) computations, the so-called FE^2 method, facilitating the incorporation of micro-mechanical material structures into macroscopic simulations. Our approach leverages deep operator networks and formulates a physics-informed operator network to approximate solutions for the representative volume element (RVE). Subsequently, homogenized quantities are computed similarly to traditional FE^2 computations, and the consistent tangent operator is derived using automatic differentiation (AD). We apply the FE-DeepONet approach to quasi-static problems in solid mechanics. The results highlight the method's ability to produce accurate solutions, even with a limited dataset during model development. Additionally, we demonstrate that an efficient implementation through state-of-the-art high-performance computing libraries and just-in-time compilation can yield multiple orders of magnitude in speedup [2].

References

[1] H. Eivazi, J.-A. Tr¨oger, S. Wittek, S. Hartmann, and A. Rausch. FE2 computations with deep neural networks: algorithmic structure, data generation and implementation. Mathematical and Computational Applications, 28(4), 2023.
[2] H. Eivazi, M. Alikhani, J.-A. Tr¨oger, S. Wittek, S. Hartmann, and A. Rausch. Enhancing multiscale simulations with constitutive relations-aware deep operator networks. arXiv:2405.13759, 2024.

Simulation meets AI: Generative Models and Adjoint Method hybrids for State Reconstruction in Complex Dynamical Systems

Sebastian Herzog[1]

[1]Gesellschaft für wissenschaftliche Datenverarbeitung mbH Göttingen

Building a representative model of a complex dynamical system from empirical evidence is a highly challenging problem. Traditionally, these models are described using systems of differential equations that capture the underlying physical laws governing the system's behavior. These equations depend on parameters that need to be optimized to fit empirical data accurately. The optimization process involves adjusting these parameters so that the model's output aligns closely with observed data. The adjoint method is a powerful technique for parameter optimization in differential equations. It is particularly effective because it can handle the optimization of a large number of parameters efficiently and reliably. This method involves solving adjoint equations that are derived from the original system of differential equations, which provides gradient information needed for optimization.

With the recent advancements in machine learning, several sophisticated engines for automatic differentiation have been developed. These engines simplify the implementation of the adjoint method by automating the derivation of adjoint equations. This automation enables researchers to apply the adjoint method to a wide range of problems without requiring extensive expertise in the underlying mathematics. However, despite its strengths, the adjoint method has a notable drawback: the quality of the optimized solution is may highly dependent on the initial parameter estimates. If the initial estimates are poor, the optimization process may converge to local minima, leading to suboptimal solutions.

In our contribution, we explore how generative models by means of artificial neural networks can be employed to mitigate this problem. Generative models have the ability to learn complex patterns from data and can be used to generate plausible initial estimates for the parameters. By leveraging these models, we can improve the initialization process, increasing the likelihood of converging to a global minimum. Furthermore, we demonstrate how it is possible to reconstruct complete state vectors from partially observable system data using these generative models. In the first case, we address the challenge of reconstructing the dynamics within a spatiotemporal chaotic 3D excitable medium. Here, we use partial observations from the surface to infer the full internal dynamics of the medium. This involves training a generative model to learn the relationship between surface observations and the underlying state of the medium.

The second case focuses on Rayleigh-Bénard convection in a turbulent regime. This physical phenomenon involves the convection of fluid in a heated system, leading to complex flow patterns. We show how to reconstruct the velocity fields from experimental, to use this data and our generative model with adjoint optimization techniques to precisely reconstruct the temperature field, which is crucial for understanding the thermal dynamics of the system. Overall, our work highlights the potential of combining generative models with the adjoint method to overcome the challenges of parameter optimization and state reconstruction in complex dynamical systems. This approach opens new avenues for improving the accuracy and reliability of models used in various scientific and engineering applications.

On modeling and simulation of acoustic cavitation

Robert Mettin[1], Christiane Lechner2, Max Koch[1], Sergey Lesnik[3], Dwayne Stephens[1], Atiyeh Aghelmaleki[1], Gunther Brenner[3]

[1]Drittes Physikalisches Institut, Georg-August-Universität Göttingen, Göttingen, Germany. Email: robert.mettin@phys.uni-goettingen.de
[2]Institut für Strömungsmechanik und Wärmeübertragung, Technische Universität Wien, Vienna, Austria
[3]Institut für Technische Mechanik, Technische Universität Clausthal, Clausthal-Zellerfeld, Germany

The phenomenon of acoustic cavitation comprises many factors on different spatial and temporal scales. Important aspects are nucleation, oscillation and collapse of bubbles, bubble translation, bubble interaction with the sound field, with neighbouring bubbles, and with objects or free surfaces. While a full, all-containing model of reasonable cost probably does not exist, the search for effective models that can capture certain essentials is still ongoing, strongly driven by applications like ultrasonic cleaning, sonochemistry, and biomedical use of ultrasound and bubbles. Numerical simulations typically focus on small, intermediate, and large spatial scales. Therefore, the presentation intends to give a brief introduction and report on selected recent approaches for simulation of individual bubbles, bubble clusters, and larger cavitating systems. Still, a coherent connection of such scales in simulation tools is mostly lacking, and the predictive power of simulations remains limited. This results in larger uncertainties even for rather “simple” observables like averaged bubble densities in the liquid. It is hoped to advance the field by connections to other branches of multi-scale problems (and solutions) in the simulation community.

InRecNet – Insect Recognition Model

Chingiz Seyidbayli[1] and Andreas Reinhardt[2]

[1]Institute for Informatics, TU Clausthal, chingiz.seyidbayli@tu-clausthal.de
[2]Institute for Informatics, TU Clausthal, andreas.reinhardt@tu-clausthal.de

The global decline in insect diversity is a key indicator of the loss of biodiversity. However, approaches to determining the insect fauna only provide a selective picture of reality, as they have so far mostly been based on time-consuming manual identification and counting methods. These require a great deal of experience and knowledge. The aim is to develop an intelligent sensor system that uses artificial intelligence methods to autonomously and self-learningly classify and count insect species on the basis of the sounds they make.

In this study, a speaker recognition-like voice recognition model is developed to identify insects from their voices. InsectSound1000 and InsectSet47 datasets are used in this study. The main goal of this work is to create a representation vector or embedding based on the audio input file. Similar to a speaker recognition or verification model, this model aims to perform the same function for insects.

A three-layer Long Short-Term Memory (LSTM) architecture is used as proof of concept. Mel-Frequency Cepstral Coefficients (MFCC) are extracted from the audio files and these features are given as input to the model. During the training of the model, a triplet loss function using anchor, positive and negative samples is used. Equal Error Rate (EER) is used as the evaluation metric.

The InsectSound1000 dataset includes 6 orders, 9 families and 12 species, while the InsectSet47 dataset includes 2 orders, 7 families and 47 species. First, the model is developed for family representation, and then the model is adapted to the species level with the fine-tuning method. This method aims to provide a more precise and accurate identification from the sounds of insects.

Several experiments are conducted to evaluate the performance of the developed model and the results are discussed. This work is an important step towards automatic identification of insect species from their sounds and has potential applications in areas such as agriculture and ecology. Furthermore, this research on insect sound recognition provides valuable information for monitoring and preserving biodiversity in nature.

Renewing Active Matter: multi-cellular assemblies and sub-cellular cytoskeleton networks

Patrick Zimmer[1,2] and Yoav G. Pollack[1,2]

1University of Göttingen, Göttingen, Germany.
2Max Planck Institute for Dynamics and Self-Organization (MPI-DS), Göttingen, Germany.

Renewing active matter deals with systems driven microscopically by growth, proliferation, de-growth and removal that lead to turnover. As opposed to the more widely explored *motile* variety of active matter, renewing active matter poses unique challenges due to the inherent injection of degrees of freedom. Dense systems of this sort such as cytoskeleton networks or multi-cellular assemblies can be viewed as soft materials, but compared to inert, thermal or motility-driven active matter can also exhibit novel features e.g. 1) in visco-elastic behaviour of the cytoskeleton or 2) in cell competition that leads to an evolution of the material composition and its properties. Here we'll present both these scenarios, the cytoskeleton work admittedly being still in it's infancy. In the multi-cellular system, simulations of stochastic (non-adversarial) mechanical competition for free space show the importance of passive matter clearance for fitness. For measuring effective forces between tracers in such a cellular active bath, unique challenges arise when probed in 1D due to the absorbing boundary condition resulting from cell removal. Applied to a real-world biological system, the numerical agent-based model seems to provide a mechanism explaining competition results in transplants of regenerating Planarian flatworms.

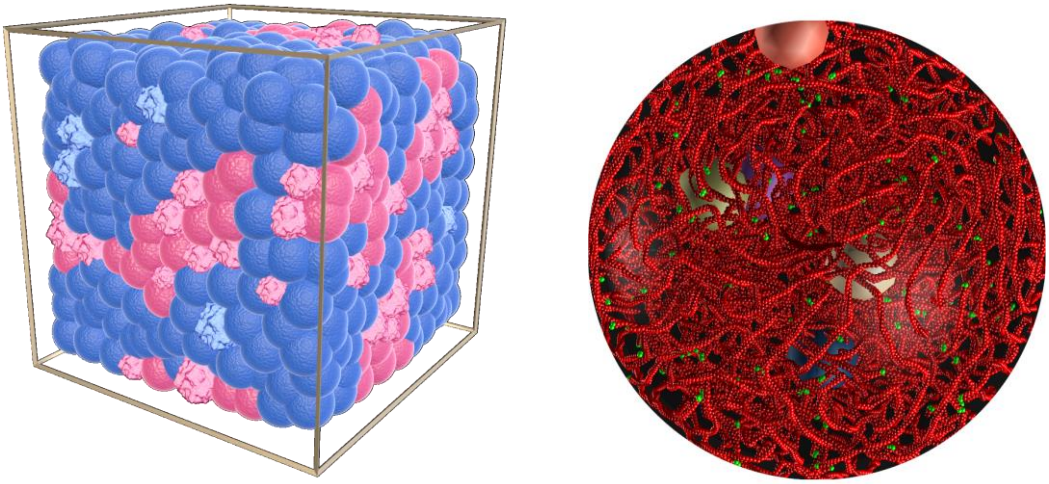


Figure 1: Left: Artist's conception. Two cell populations (blue and pink) that are renewing through growth, division, death, *and degradation* compete for limited space. Right: Cytosim simulation. Actin filaments (red) can undergo turnover by actively polymerizing, de-polymerizing, getting severed and nucleating. Beads allow for micro-rheology measurements.

Modeling actin and synapse geometry

Mitha Thomas[1] and Michael Fauth[1]

[1]Third Institute for Physics, Georg-August University Göttingen

Synapses and the adjustment of their transmission efficacies are believed to form the biophysical substrate for long-term memory. For excitatory synapses, which typically reside on dendritic spines, the transmission efficacy is correlated with the size of the spine and the postsynaptic density. Interestingly, these morphological properties have been shown to undergo significant spontaneous fluctuations, which might have an impact on memory. Therefore, we need a deeper understanding of their origin and nature of these fluctuations.

We derived a biophysical model describing the dynamic of dendritic spine geometry based on the scaffolding protein actin. This protein forms branched filament networks that undergo continuous reorganization and treadmilling, which, in turn, gives rise to expansive forces within the spine. The balance between these expansive forces and the counteracting forces from the membrane determines the membrane deformation. The dynamic of actin filaments, which depends on a multitude of actin-binding proteins like cofilin or ARP2/3 as well as on the counterforce of the membrane, is described as a Markov process for each filament network.

Through these feedback mechanisms between actin, forces and spine geometry, the model selforganizes into a stationary state around which it fluctuates which is statistically equivalent to that of experimentally imaged spines on a timescale of minutes. Assessing the functional significance of such fluctuations, we show that self-organization brings actin close to a critical state, at which it exhibits quick and long-lasting reactions to parameter perturbations as for example during plasticity.

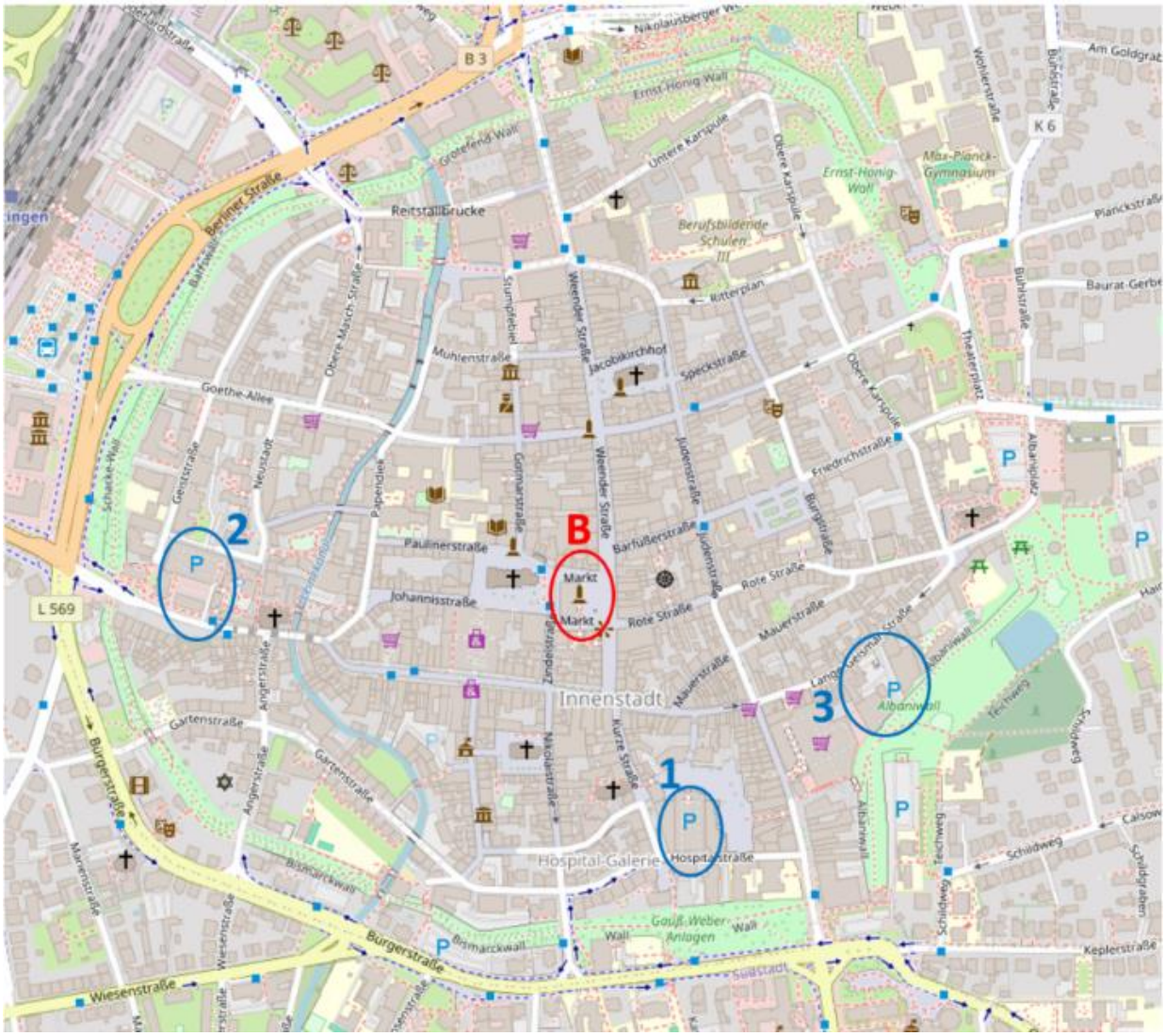
As a next step, we therefore modeled the geometrical changes during long-term potentiation emerging from perturbations in the actin-binding protein concentrations. In particular, we ask whether actin and spine geometry can serve as transient memory of the plasticity event, corresponding to the synaptic tag. We demonstrate that memory on this timescale requires the introduction of a stable actin pool with a slower treadmilling dynamic.

Taken together, our model can serve as a tool to determine the consequence of experimentally measurable perturbations in molecular dynamics onto the long-term dynamic of spine geometry and, ultimately, also the synaptic weight.

Conference Dinner

The conference dinner on Thursday evening will take place in restaurant “Bullerjahn” in Göttingen city center. Since there is no conference fee, you have to pay for the conference dinner yourself.

Address:
Markt 9
37073 Göttingen



SWZ strategy discussion

This document is directly editable online via:

https://tu-c.de/swzforschungsfelder

(Password: “**Workshop**”)

Basis for discussion of the update of the fields of research of SWZ:

Das SWZ befasst sich sowohl mit der Weiterentwicklung von Simulationsmethoden als auch mit deren Anwendung in verschiedenen Bereichen in Mathematik, Informatik, Physik und den Ingenieurwissenschaften.

Simulationsmodelle zur Beantwortung von konkreten Fragen werden in allen Bereichen der Industrie, der Wissenschaft sowie für viele gesellschaftliche Fragestellungen eingesetzt. Das SWZ erforscht und entwickelt dafür geeignete Methoden und Werkzeuge und bietet diese aktiv den jeweiligen Nutzern an. Dabei stehen einerseits empirische und modellbasierte Ansätze und andererseits datenbasierte Ansätze wie Methoden der Künstlichen Intelligenz und des High Performance Computings im Fokus.

Empirische und modellbasierte Ansätze beschreiben die Entwicklung eines Systems auf Basis von Gesetzmäßigkeiten, z.B. der Physik. Materialsimulationen zeichnen sich so durch eine Vielzahl verschiedener Simulationsmethoden aus, welche auf die jeweilige Problemklasse und die entsprechenden Längen- und Zeitskalen zugeschnitten sind. Prognostische Verfahren basieren auf der Analyse großer Datenmengen.

Die aktuellen Projekte am SWZ gliedern sich in die im Folgenden dargestellten Bereiche. Die Auflistung der Forschungsgebiete stellt dabei eine Momentaufnahme dar und kann und wird durch zukünftige Projekte ergänzt.

Simulation und Optimierung von Netzen

Die Simulation ist heute eine der wichtigsten und in vielen Fällen einzig praktikablen Techniken zur Analyse und Optimierung von großen Netzen. Telekommunikationsnetze, Verkehrs-/Logistiknetze und Energienetze haben vieles gemeinsam. Die Komplexität der Netze mit ihren vielen parallel existierenden Knoten und den Strömen zwischen den Knoten ist schwer überschaubar und oft mit anderen Techniken als Simulation nicht beherrschbar. Das tatsächliche Verhalten eines solchen Netzes unterscheidet sich oft von dem vermuteten Verhalten. Der Aufbau, Betrieb, Modifikation und Optimierung solcher Netze stellt in der Regel eine Infrastrukturaufgabe dar, die mit erheblichen Kosten verbunden ist. Um hier Fehlentwicklungen zu vermeiden, wird vor einer physischen Installation die Simulation als wichtigstes Hilfsmittel eingesetzt, um die Eigenschaften eines Netzes, das Verhalten, die kritischen Leistungskenngrößen und Parameter in einem frühen Stadium zu ermitteln. Die 2005 in Kraft getretene EU-Verordnung z.B. zu Ausgleichszahlungen an Fluggäste bei Annullierungen oder großen Verspätungen (EG 261/2004) unterstreicht die Notwendigkeit geeigneter Verfahren und Systeme für den praktischen Einsatz.

Im Kontext der Industrie 4.0 haben sich mittlerweile sogenannte Digitale Zwillinge, mit denen verschiedene Aspekte der realen Produktion sowohl im Vorfeld von Bau und Inbetriebnahme als auch im laufenden Betrieb analysiert und optimiert werden können, etabliert. Im Rahmen der Forschung am SWZ werde die entsprechenden Methoden zur Modellierung und Simulation weiträumig vernetzter Produktions- und Logistikprozesse weiterentwickelt und zusammen mit Industriepartnern praktisch erprobt.

Simulation von Materialien

Die Fortschritte der Materialwissenschaften haben seit jeher den Entwicklungsstand einer Gesellschaft definiert. Materialwissenschaften sind gerade in der deutschen Industrielandschaft eines der zentralen Themen, welche die Grundlage für viele Innovationen in anderen Industriezweigen liefern.

In den Materialwissenschaften hat sich bereits eine stark interdisziplinäre Arbeitsweise herausgebildet, welche in den stark überlappenden Bereichen „Computational Materials Science“, „Computational Physics“ and „Computational Chemistry“ ausgeprägt ist. Simulationen haben sich in den Materialwissenschaften und den benachbarten naturwissenschaftlichen Disziplinen zu einem lebendigen und forschungsstarken Wissenschaftszweig herausgebildet, der vermehrt auch von der Industrie wahrgenommen und aktiv gefördert wird.

Probleme der Materialwissenschaften sind sehr vielfältig und spielen sich typischerweise auf unterschiedlichsten Längen- und Zeitskalen ab. Deshalb zeichnet sich das Feld der Materialsimulationen durch eine Vielzahl verschiedener Simulationsmethoden aus, welche auf die jeweilige Problemklasse zugeschnitten sind:

Auf der kleinsten Längenskala werden in so genannten ab-initio Simulationen atomare Prozesse parameterfrei auf der Grundlage von Naturgesetzen simuliert. Diese quantenmechanischen Methoden erfordern meistens Hochleistungsrechner, erlauben aber vielfältige und quantitative Aussagen zu treffen. Ein solches Programmpaket wird in Clausthal entwickelt und vertrieben.

Auf der makroskopischen Längenskala wird das Material als ein Kontinuum betrachtet, dessen Verhalten von Materialparametern bestimmt wird, die entweder aus dem Experiment bekannt oder durch grundlegendere Simulationen bestimmt wurden. Weil die Simulationstechniken hier weitgehend einheitlich sind, kommen besonders kommerzielle Programmpakete zum Einsatz. Das Hauptinteresse richtet sich hier auf die Modellierung des Problems und die Bestimmung der dabei verwendeten Parameter und Zustandsgleichungen, sowie die Verifikation und die Visualisierung der Resultate.

Zwischen diesen Polen befinden sich eine Vielzahl weiterer Methoden die hier nur einige als Stichworte genannt werden sollen: Monte-Carlo Methoden, Molekularmechanik, Molekulardynamik, Phasenfeldtheorien, Mikrostruktursimulation von Versetzungsnetzwerken und Korngrenzen.

Eine der „Grand Challenges in Computational Materials Science“ ist daher die Multiskalensimulation, die im Idealfall von der ab-initio Simulation bis zur Simulation von Umformprozessen und Herstellungsverfahren reicht. Diese Herausforderung wird einerseits dadurch angegangen, dass Simulationsparameter gezielt von den mikroskopischen Simulationen zu den makroskopischen Simulationen durchgereicht werden. Andererseits werden unterschiedliche Simulationsmethoden in eine einheitliche Simulationsumgebung integriert, um Effekte zu beschreiben, bei denen unterschiedliche Längen- und Zeitskalen nicht mehr entkoppelt werden können. Diese Aktivitäten erfordern die Zusammenarbeit unterschiedlicher Wissenschaftsdisziplinen und profitieren von Zusammenschlüssen, wie sie im Simulationswissenschaftlichen Zentrum geplant sind.

Im Gegensatz zu etlichen anderen Anwendungen von Simulationsverfahren sind Simulationen im Bereich der Materialwissenschaften sehr häufig dadurch gekennzeichnet, dass sie alle verfügbaren, informationsverarbeitenden Ressourcen bis an die Grenzen ausschöpfen müssen, um verwertbare Ergebnisse zu erzielen. Fragen der algorithmischen Komplexität und der Effizienz von Implementierungen sind daher für Fortschritte der Simulationsmethoden in diesem Teilgebiet von entscheidender Bedeutung.

Da Optimierung und Charakterisierung von Materialien mit großen Datenmengen in verschiedenen Formaten verbunden sind, werden zunehmend Methoden der Künstlichen Intelligenz zur Analyse verwendet. Diese Methoden können zur Erzeugung synthetischer Daten eingesetzt werden, wenn Analytik und konventionelle Modellierung an ihre Grenzen stoßen. In den letzten Jahren haben sich daher Machine-Learning-Methoden zur Vorhersage von Struktur-Eigenschafts-Beziehungen und zur Materialentwicklung etabliert. Dabei hängt jedoch die Vorhersagekraft von der Verfügbarkeit großer Datensätze ab, weshalb sich einige Aspekte immer noch besser per Simulation beschreiben lassen. Das SWZ bringt diese Kompetenzen in verschiedene Anwendungsfelder der Materialwissenschaft und Werkstofftechnik ein.

Simulation soziotechnischer Systeme

Die Echtzeitsteuerung von Mensch-Maschine-Teams in der Fertigung und im Dienstleistungssektor befasst sich hauptsächlich mit der Koordination von Plänen und Aktionen der Teammitglieder während der gemeinsamen Bearbeitung und Verarbeitung einzelner Vorgänge. Im Fokus steht hierbei eine integrierte Betrachtung der Effizienz des soziotechnischen Gesamtsystems und der Zufriedenheit und Sicherheit des Menschen.

Für eine eng-gekoppelte Zusammenarbeit zwischen Menschen und Maschinen ist es erforderlich, dass sowohl menschliche als auch maschinelle Mitglieder eines Teams ein gemeinsames Verständnis von ausgeführten Aktionen haben.

Ein weiterer wichtiger Faktor ist das Vertrauen zum Kollaborationspartner – sowohl vom Menschen in die Maschine als auch umgekehrt. Nur mit Vertrauen kann eine Verlässlichkeit von Verhalten erreicht werden, wodurch das volle Potential einer Kollaboration erst erreicht werden kann. Menschen können einer Maschine nur vertrauen, wenn die Maschine bekanntermaßen gut getestet ist, so wie die Zusammenarbeit zwischen Menschen schwierig ist, wenn einer der Beteiligten einen schlechten Ruf hat. Die Modellierung von Vertrauen aus der Perspektive der Maschine ist das messbare Gesamtergebnis der Auswertung von Variablen, die den menschlichen Zustand und das menschliche Verhalten beschreiben.

Der Entwurf von Interaktionsmodellen für die Mensch-Maschine-Zusammenarbeit erfordert einen interdisziplinären Ansatz: Es müssen sowohl Vertrauens- und Intentionsmodelle integriert werden als auch die Interaktion anpassungsfähig und mit einem hohen Grad an Automatisierung im Engineering-Prozess gestaltet werden.

Ein kollaborativer Roboter in einem Team sollte in der Lage sein, das Vertrauen seines menschlichen Partners in ihn zu erkennen und sicherzustellen, dass dieser menschliche Partner seinen Fähigkeiten nicht zu sehr vertraut und ihn für Aufgaben einsetzt, für die er nicht konzipiert wurde. Sie sollte den Partner auch davon abhalten, sich selbst oder die Gesamtaufgabe zu gefährden. Dies spiegelt die Notwendigkeit einer dynamischen Vertrauenskalibrierung während der menschlichen Zusammenarbeit mit einer autonomen Maschine wider.

Die Erfassung physiologischer Parameter hat sich als gut geeignet erwiesen, um Informationen über die kognitiven Bedingungen des Menschen abzuleiten, und ist äußerst relevant für die Zuweisung eines Vertrauensniveaus. Die Erfassung solcher Phänomene wird jedoch nicht nur durch den Grad an Akzeptanz und potentieller Beeinträchtigung menschlicher Handlungen begrenzt, sondern auch durch die monetären Kosten für die Instrumentierung der Arbeitsplätze mit der Sensor-Infrastruktur, um die erforderlichen Daten zu erfassen.

Um fundierten Entscheidungen treffen zu können, muss die Maschine nur den aktuellen Zustand des menschlichen Teamkollegen modellieren, sondern auch kurzfristig zuverlässige

Vorhersagen über die Handlungen, Pläne und sogar Absichten des Teamkollegen treffen. In diesem Zusammenhang sind die Modellierung und das Antizipieren von Bewegungen des menschlichen Körpers und Laufwegen von entscheidender Bedeutung. Neben den Bewegungen der Hand und des Kopfes sind auch Armbewegungen im Zusammenhang mit der sicheren Mensch-Maschine- Zusammenarbeit z.B. bei Montage- oder Demontageprozessen von Bedeutung, ebenso wie die Laufwege der Menschen.

Simulation in der Physik

… neben Theorie und Experiment dritte Säule...

Die Strömungsmechanik ist ein „Klassiker“ der Simulationen in der Physik, den Ingenieurdisziplinen sowie bei vielen interdisziplinär angesiedelten Problemstellungen. Als Beispiele seien das Verhalten von Galaxien, die Luftströmung um Automobile oder das Innere von lebenden Zellen genannt. Um auf aufwändige und teure Experimente – falls diese überhaupt möglich sind – mindestens teilweise verzichten zu können, werden die untersuchten Systeme simuliert. Auf Basis der seit langem bekannten Gleichungen gilt es dann i.d.R., mangels analytischer Lösung dieselbe auf numerischem Wege zu finden. Da Komplexität und Umfang der Berechnungen aber enorm sein können, muss man häufig effektive numerische Verfahren oder/und vereinfachende Modelle einsetzen, so dass die Aufgabenstellung überhaupt behandelbar wird. Daher gehen mit den steigenden Rechenleistungen auch weiterhin Fortschritte in der Modellbildung und bei Algorithmen einher, und auch KI ist ein Thema. Aktuell werden z.B. Mehrphasenströmungen und Kavitation in Simulationen behandelt, um Probleme wie die Erosion von Schiffspropellern, die Reinigung von Halbleitern, Poration von Zellwänden oder neuartige pharmakologische Methoden zu simulieren.

ML supported simulation in deep drilling technology

Gunther Brenner[1]

[1]Institut für Technische Mechanik, TU Clausthal

Deep drilling technology is particularly important in connection with the energy and heat transition. This technology has long been established in the field of fossil fuels (gas, oil). Today, deep drilling technology is a basic prerequisite for the development of geothermal, i.e. sustainable energy sources. However, the development of geothermal sources for heat supply poses a number of special challenges. The value added in the context of geothermal energy is significantly lower than for fossil fuels. Geothermal reservoirs must be developed in the vicinity of consumers, resulting in increased safety requirements.

The presentation will give an overview of these challenges and possibilities to gain a better understanding of the processes during drilling by means of simulation. In this context, not only numerical calculations but also simulation through physical experiments should be considered. Increasingly, data-driven models are being used for evaluation and modeling. The lecture will present initial results on specific applications.

Digitization in Materials Science - Challenges in Multiscale Modeling of Oxygen-Free Production

Nina Merkert[1]

[1]Simulation Science Center Clausthal-Göttingen

Simulations in material science often require a combination of different methods that act on different length scales. This multiscale character is caused by the strongly heterogeneous microstructures present in virtually all materials, ranging from crystal defects at the atomistic level up to macroscale pores. The microstructure has a significant impact on product manufacturing, necessitating adjustments in engineering processes and novel approaches to data management. This requires an in-depth examination of the process of data generation as well as the information flows and data exchange between different production methods.

In this talk, I will present the research data management strategy of the working group oxygen-free production of the CRC 1368. Oxygen-free production techniques can lead to high-quality, metallurgically-bonded compounds. In this context, the consideration of the interphase phenomena during the joining process under oxidation-free conditions is one of the most essential factors influencing the product quality. The Data Management System processes and manages a vast quantity of experimental and simulation data. By mapping and transferring the outcomes, a crossscale model for the fundamental comprehension of joining technology processes will be developed.

Atomistic simulations of the shock and spall behavior of the refractory high-entropy alloy HfNbTaTiZr

Daniel Thürmer[1]

[1]Simulation Science Center Clausthal-Göttingen

Atomistic simulations of the shock and spall behavior of the refractory high-entropy alloy HfNbTaTiZr were carried out for single-crystalline samples, shocked along the [001] direction. The initial compression leads to reduced dislocation activity and a bcc → hcp transformation in some regions of the sample. Upon release, hcp transforms back to bcc, and twins are formed in the bcc phase. Further release leads to dislocation activity at the twin boundaries and some limited dislocation activity inside the nanograins generated by twinning. Some fcc phase appears at large tensile stress, together with disordered amorphous regions where voids nucleate and lead to spall. The fracture surfaces follow the twin boundaries set up in the late compression phase. The spall strength is similar to the one found in simulations of other bcc metals at similar strain rates, and we observe some differences between the spall strength from the local atomic stress and the one deduced from the back surface velocity. Similar simulations for HfNbTaZr show the same qualitative behavior, with twins and reduced dislocation activity, but without phase transformations.

Engineered compounds for the recovery of critical elements from slags: melt characteristics of Li5AlO4, LiAlO2 and LiAl5O8

Iyad Alabd Alhafez[1]

[1]Simulation Science Center Clausthal-Göttingen

Engineered artificial minerals (EnAM) are designed scavenger compounds with high potential for the recovery of critical elements from slags. $LiAlO_2$ is a promising EnAM for the recovery of lithium from Li-ion battery pyrometallurgical processing. It can be obtained through the addition of aluminum to the recycling slag melt. The formation of compounds in the slag is governed by phase separation. Depending on the temperature, "solid-melt" or melt "liquid-liquid" separation can occur. The separation gives rise to gradients in composition, ion diffusivity and viscosity. The latter two parameters are of high importance as they influence compound formation from slags which in large parts is kinetically controlled. Accordingly, in this study we determine high temperature properties spanning from below to above the liquidus temperature of three stoichiometric LiAl Oxides: Li_5AlO_4 $LiAlO_2$ and $LiAl_5O_8$ using molecular dynamics (MD) simulation. The obtained viscosity is validated experimentally, from compounds synthesized via the sol-gel route. The Li^+ ion exhibits the largest diffusivity. They are quite mobile already below the liquidus temperature. The other ions Al^{3+} and O^{2-} do not move considerably at that temperature. The diffusivity of Li^+ is largest in the Li-rich compound Li_5AlO_4. The viscosity is lower the higher the Li-content.