Working Group on Physics, Modern IT and Artificial Intelligence Arbeitskreis Physik, moderne Informationstechnologie und Künstliche Intelligenz (AKPIK)

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Overview of Invited Talks and Sessions

(Lecture hall MAR 0.002; Poster B)

Sessions

AKPIK 1.1–1.6	Tue	9:30–11:00	MAR 0.002	**Reservoir Computing & Neural Networks**
AKPIK 2.1–2.5	Wed	15:00–16:15	MAR 0.002	**Machine Learning & Physics**
AKPIK 3.1–3.9	Thu	11:00–14:30	Poster B	**Poster**

AKPIK 1: Reservoir Computing & Neural Networks

Time: Tuesday 9:30–11:00 Location: MAR 0.002

AKPIK 1.1 Tue 9:30 MAR 0.002

Minimal Reservoir Computing — •Haochun Ma[1], Davide Prosperino[1], and Christoph Räth[2] — [1]Allianz Global Investors, risklab, Seidlstraße 24, 80335, Munich, Germany — [2]Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für KI Sicherheit, Wilhelm-Runge-Straße 10, 89081 Ulm, Germany

Reservoir computers are powerful machine learning algorithms for predicting nonlinear systems. However, the traditional reservoir computer uses random matrices to define the underlying recurrent neural network and has a large number of hyperparameters to optimize.

Here, we show that a few simple modifications to the traditional reservoir computer architecture, which eliminate randomness and minimize computational resources, lead to significant and robust improvements in short- and long-term predictive performance compared to similar models, while requiring minimal amount of training data. Specifically, the adjacency matrix of the reservoir becomes a block diagonal matrix, where each block is the same matrix with all elements being one. Further, we omit the nonlinear activation function. The nonlinearity is only introduced by also taking higher powers of the reservoir response. Thus, this new architecture open new avenues to explainable and interpretable reservoir computing.

For certain parameterizations, we find that the predictions are accurate for more than 10 Lyapunov times and that ordinary least squares regression directly on the embedded data can predict the long-term climate of chaotic systems [1].

[1] H.Ma et al., Sci. Rep., 13, 12970 (2023)

AKPIK 1.2 Tue 9:45 MAR 0.002

Novel implementations for reservoir computing – from spin to charge — •Atreya Majumdar[1], Karin Everschor-Stte[1], Katharina Wolk[2], and Dennis Meier[2,3] — [1]Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany — [2]Department of Materials Science and Engineering, Norwegian University of Science and Technology (NTNU), Trondheim 7034, Norway — [3]Center for Quantum Spintronics, Norwegian University of Science and Technology (NTNU), Trondheim 7034, Norway

Magnetic and ferroelectric materials are emerging as promising candidates for unconventional computing and next-generation information technology. We review and explore the potential of nanoscale topological textures, focusing on magnetic skyrmions and ferroelectric domain walls, for use in reservoir computing [1] a scheme that allows transforming non-linear tasks into linearly solvable ones. We highlight the essential characteristics needed for physical reservoirs, outlining the advantages of topological textures, such as the increased complexity and flexible input and output options. We provide insights into how topological textures in magnetic and ferroelectric systems can serve as an avenue for enhancing reservoir computing and, more generally, broadening the scope of in-materio computing.

[1] K. Everschor-Sitte, A. Majumdar, K. Wolk, D. Meier, arXiv:2311.11929

AKPIK 1.3 Tue 10:00 MAR 0.002

Analyzing phase transitions in minimal reservoir computers — •Davide Prosperino[1], Haochun Ma[1], and Christoph Räth[2] — [1]Allianz Global Investors, risklab, Seidlstraße 24-24a, 80335, Munich, Germany — [2]Deutsches Zentrum für Luft- und Raumfahrt (DLR), Institut für KI Sicherheit, Wilhelm-Runge-Straße 10, 89081 Ulm, Germany

Minimal reservoir computers are powerful machine learning algorithms that can accurately predict nonlinear systems [1]. They differ from traditional feedforward neural networks by not relying on randomness but instead utilizing linear optimization, which enables them to operate on small training datasets and requires minimal computational resources.

Additionally, they can make accurate predictions for over ten Lyapunov times with certain parameterizations. However, we discovered that for certain parametrizations, the prediction fails. With only a few parameters, the phase transition between various parameterizations can be analyzed to comprehend the reasons behind the success of a prediction. We do that by analyzing the reconstructed, underlying equations.

[1] H. Ma, D. Prosperino, et al., Sci. Rep., 13, 12970 (2023)

AKPIK 1.4 Tue 10:15 MAR 0.002

Image reconstruction with diffusion models for accelerated magnetic resonance imaging — •Christine Müller[1], Vanya Saksena[2], Florian Knoll[2], and Bernhard Kainz[1] — [1]Image Data Exploration and Analysis Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Computational Imaging Lab, Friedrich-Alexander-Universität Erlangen-Nürnberg

Magnetic resonance imaging (MRI) is a widely used non-invasive imaging technique in medical practice. However, conventional MRI acquisitions are often time-consuming, limiting their applicability in clinical settings. Accelerated MRI techniques reduce scan time but come at the expense of image quality. Diffusion models are a recent promising class of generative models for image reconstruction in MRI [1,2]. These models learn to generate high-quality images from undersampled MRI data by gradually denoising a noisy image.

In this work, we evaluate the performance of a score-based diffusion model that was trained on brain MRI data from the publicly available fastMRI dataset [3]. It employs a predictor-corrector sampling step and combines parallel imaging and compressed sensing techniques. A learned score function is utilized as a prior to guide the reconstruction process, enabling the generation of realistic content, especially at high acceleration rates. Diffusion models offer the potential to improve the quality of reconstructed images and reduce scan time, making MRI more accessible and efficient.

[1] DOI: 10.1016/j.media.2022.102479, [2] DOI: 10.1016/j.media.2023.102846, [3] DOI: 10.1148/RYAI.2020190007

AKPIK 1.5 Tue 10:30 MAR 0.002

Performance of RBM neural quantum states from the perspective of the quantum geometric tensor — •Sidhartha Dash[1], Filippo Vicentini[2,1], Michel Ferrero[2,1], and Antoine Georges[1,2,3] — [1]Collège de France, Université PSL, 11 place Marcelin Berthelot, 75005 Paris, France — [2]CPHT, CNRS, École polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France — [3]Center for Computational Quantum Physics, Flatiron Institute, New York, New York, 10010, USA

There have been a lot of recent advances in using artificial neural networks, as variational ansätze (Neural quantum states), to approximate the ground states of quantum systems. Various neural network architectures including RBMs, RNNs, CNNs, and Transformers have been successfully used to approximate the ground states of many quantum spin models with a reasonable accuracy. However, the practical limit of the representation power of such ansätze is far from being understood. The universal approximation theorems only guarantee that the RBM can represent any distribution with an arbitrary accuracy, given a sufficient number of hidden units which is exponential in system size. In this work, we systematically study the accuracy of RBMs for representing the groundstate of spin-1 models. We use the quantum geometric tensor at convergence to characterize the performance of the ansatz for various spin-1 models, and for various densities of the network.

AKPIK 1.6 Tue 10:45 MAR 0.002

Physics-Informed Deep Learning to Couple Reactive Diffusion and Swelling in Cellulose-based Porous Media — •Alexandra Serebrennikova[1], Maximilian Fuchs[1], Raimund Teubler[2], and Karin Zojer[1] — [1]Institute of Solid State Physics, TU Graz, Graz, Austria — [2]Institute of Analytical Chemistry, TU Graz, Graz, Austria

Simulating the reactive diffusion of fluids through porous media presents significant challenges due to the intricate geometries of real-world systems, particularly when the porous media itself undergoes changes, such as swelling of the solid matrix. Traditional numerical solvers often struggle to represent these complex details accurately and feasibly. Based on state-of-the-art extended physics-informed neural networks (PINNs), this contribution focuses on creating a mesh-free modeling framework for studying the reactive transport of volatile organic compounds (VOCs) through the complex microstructure of paper. PINNs serve us to implicitly incorporate the experimentally observed evolution of geometrical features of paper matrix into the formulation of the governing partial differential equations. This approach enables to study the spatio-temporal evolution of VOC concentrations in the porous environment of paper, while the geometry of the material

dynamically adapts itself through swelling or shrinking as response to the current state of adsorption.

To our knowledge, this is the first contribution that applies PINNs to consider adaptive geometries during transport.

AKPIK 2: Machine Learning & Physics

Time: Wednesday 15:00–16:15 Location: MAR 0.002

AKPIK 2.1 Wed 15:00 MAR 0.002

Bringing long-ranged interactions to the JAX ecosystem with the multilevel summation method — •Florian Buchner[1], Johannes Schörghuber[1], Jesús Carrete[2,1], and Georg K. H. Madsen[1] — [1]Institute of Materials Chemistry, TU Wien, 1060 Vienna, Austria — [2]Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza, 50009 Zaragoza, Spain

Despite the tremendous success of machine-learned force fields (MLFFs), their extension beyond the locality approximation remains a field of active research. In constructing such MLFFs, the efficient (ideally with linear scaling) evaluation of pairwise long-ranged interactions is a ubiquitous requirement. It is routinely solved by well-established algorithms such as Ewald summation.

While implementations of such algorithms are readily available, they tend not to interface well with modern machine-learning environments and workflows. This includes Google's JAX framework, which is proving transformative to machine-learning research by providing high performance and general-purpose automatic differentiation.

Here, we present a JAX-based implementation of the multilevel summation method (MSM) [D. J. Hardy *et al.*, J. Chem. Phys. 144, 114112 (2016)], a powerful linearly scaling algorithm for pairwise long-ranged interactions. Its notable features include support for mixed boundary conditions and freedom from artefactual force discontinuities encountered in competing methods. We introduce the basics of the MSM, discuss our design and implementation strategy, and highlight example applications.

AKPIK 2.2 Wed 15:15 MAR 0.002

Atomic Graph-based Symmetry Search for Enhancing Machine Learning Force Fields Architectures — •Anton Charkin-Gorbulin[1,2], Igor Poltavsky[1], Alexandre Tkatchenko[1], Claudio Quarti[2], and David Beljonne[2] — [1]University of Luxembourg, Luxembourg, Luxembourg — [2]University of Mons, Mons, Belgium

Machine-learning force fields (MLFF) show high accuracy and efficiency for modeling the potential energy surfaces of molecules, materials, and interfaces. However, the performance of MLFFs greatly depends upon incorporating the physical symmetries. Finding all relevant symmetries becomes a challenging task for large system sizes. Here, we develop a data-driven method based on molecular graphs to reveal relevant permutational symmetries and distinguish atoms with different chemical environments in molecules and materials.

The method was applied to improve the performance of the kernel ridge regression (KRR) model and the message-passing neural network (MPNN). KRR model, enhanced with extracted symmetries, demonstrates superior accuracy, enabling comprehensive investigations of complex systems like the 1,8-naphthyridine/graphene interface at finite temperatures. MPNN was enhanced by expanding atomic species using the extracted distinctive chemical environments, resulting in improved accuracy for $CsPbI_3$ slab systems, particularly notable with large training sets. Overall, this research underscores the critical role of symmetries in advancing MLFFs for complex systems, enabling further advances in atomistic simulations.

AKPIK 2.3 Wed 15:30 MAR 0.002

Combining genetic algorithm and compressed sensing for features and operators selection in symbolic regression — •Aliaksei Mazheika[1], Sergey V. Levchenko[2], and Luca M. Ghiringhelli[3,4] — [1]Technische Universitaet Berlin, DE — [2]Moscow, RU — [3]The NOMAD Laboratory at the Fritz Haber Institute and Humboldt University, Berlin, DE — [4]Friedrich-Alexander University, Erlangen, DE

The symbolic inference method SISSO (Sure-Independence Screening and Sparsifying Operator) has recently found a broad application in materials science. It performs regression or classification by adopting compressed sensing for the selection of an optimized subset of features and mathematical operators out of a given set of candidates. However, SISSO becomes computationally unpractical when the set of candidate features and operators exceeds the size of few tens. Here we combine SISSO with a genetic algorithm (GA) for the global search of the optimal subset of features and operators. We test GA-SISSO for the search of predictive models of perovskites lattice parameters, and demonstrate that our method efficiently finds more accurate models than the original SISSO. GA-SISSO was also applied for the search of the model for prediction of CO_2 adsorption energies on semiconductor oxides. The model learned by GA-SISSO has much higher accuracy compared to previously discussed models based on the O 2p-band center. The statistical analysis of contributions of all features to the learned models shows that, besides the O 2p-band center, the electrostatic potential above adsorption sites and surface formation energies are key features.

AKPIK 2.4 Wed 15:45 MAR 0.002

PSeudocode Projective Simulation (PS^2) — •Marius Krumm and Hans J. Briegel — University of Innsbruck, Institute for Theoretical Physics, Technikerstr. 21a, A-6020 Innsbruck, Austria

The rise of deep learning has enabled significant progress in technology and science. However, the opaque oracle-like nature of artificial neural networks severely limits their potential to discover new qualitative scientific insights. This motivates the exploration of methods from eXplainable AI (XAI) that allow to understand the reasoning process of accurate predictions. In this talk, I present a new XAI method called PSeudocode Projective Simulation (PS^2) which represents chains-of-thought in the form of pseudocodes. Here, a thought is modeled as a small data processing module acting on the agent's memory, which can be a trainable neural network. These subroutines are selected in a trainable random walk, making our method an extension of Projective Simulation. On a technical level, methods from hierarchical and safe reinforcement learning are adapted and integrated into our setting. These modified methods help to model domain knowledge about the nature of the thoughts and the environment. The framework is applied numerically to the Highway-Env.

AKPIK 2.5 Wed 16:00 MAR 0.002

Humans in the loop for more trustworthy Bayesian optimization of materials — •Armi Tiihonen[1], Louis Filstroff[2], Petrus Mikkola[1], Emma Lehto[1], Samuel Kaski[1,3], Milica Todorović[4], and Patrick Rinke[1] — [1]Aalto University, Espoo, Finland — [2]ENSAI, CREST, Rennes, France — [3]The University of Manchester, Manchester, United Kingdom — [4]University of Turku, Turku, Finland

Bayesian optimization (BO) is a machine learning method for global optimization of black-box functions, e.g. the composition of perovskite materials for more stable solar cells. BO can be coupled to automated sample preparation and characterization pipelines, which introduces the challenge of ensuring sufficient sample quality during the optimization. Low quality samples are hard to detect automatically, but could obscure the optimization process. To make automated materials optimizations more robust and trustworthy, we add humans into the BO loop (HITL) as an additional data source. We implemented three HITL schemes, two based on data fusion and one on multifidelity BO. They query human opinion on sample quality only when necessary and guide the sampling away from composition regions with a lot of low-quality samples. We tested them in simulations based on previously obtained experimental perovskite data. Our data fusion HITL BO queries from humans on average 7% of the samples when the run is repeated 25 times. This leads to only 2% of low quality samples, in contrast to the 25% with the reference method without humans. Thus, HITL ensures more consistent sample quality during BO.

AKPIK 3: Poster

Time: Thursday 11:00–14:30 Location: Poster B

AKPIK 3.1 Thu 11:00 Poster B

A surrogate model for graphene-based conductor materials and the creation of an ontology-based digital twin — •Fabian Teichert[1,2,3], Philipp Schulze[4,5], Florian Fuchs[1,2,3], Martin Stoll[4], and Jörg Schuster[1,2,3] — [1]Fraunhofer Institute for Electronic Nano Systems (ENAS), Chemnitz, Germany — [2]Center for Microtechnologies, Chemnitz University of Technology, Chemnitz, Germany — [3]Center for Materials, Architectures and Integration of Nanomembranes (MAIN), Chemnitz University of Technology, Chemnitz, Germany — [4]Faculty of Mathematics, Chemnitz University of Technology, Chemnitz, Germany — [5]Institute of Mathematics, Technische Universität Berlin, Berlin, Germany

(1) We developed a surrogate model for graphene-based conductor materials using Gaussian process regression. The material of interest is a stack of layers of graphene flakes. The results of previously performed nodal analysis have been used to obtain a model for calculating in-plane and out-of-plane conductivities much faster. We present results depending on various material parameters like flake size, packing density, flake conductivity, and inter-layer conductivity.
(2) Recently the „Plattform MaterialDigital“ (www.materialdigital.de) started to facilitate digital twins in material science, i.e. the creation of an ontology-based data storage for the digital representation of (new) materials and their properties in relation to key processing steps. We participate in this and present an ontology specialized to graphene-based conductor materials, which we fill with simulation data as well as laboratory data.

AKPIK 3.2 Thu 11:00 Poster B

Estimating sliding drop width using recurrent neural networks — •Sajjad Shumaly[1], Fahimeh Darvish[1], Xiaomei Li[1], Oleksandra Kukharenko[1], Werner Steffen[1], Yanhui Guo[2], Hans-Jürgen Butt[1], and Rüdiger Berger[1] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, D-55128, Mainz, Germany — [2]Department of Computer Science, University of Illinois Springfield, Springfield, IL, USA

Recording videos serves as a technique for monitoring objects and researching physical phenomena through image processing. Challenges emerge when dealing with soft matter objects such as sliding drops, which exhibit variations in size. Adding additional cameras or mirrors to track drop size variation from the front view can be inconvenient and limit the field of view. This limitation can impede a comprehensive analysis of sliding drops, especially when dealing with scenarios that entail surface defects. Our study explores the use of various regression and multivariate sequence analysis models to estimate drop/solid contact width (drop width) solely from side-view videos. The long short term memory (LSTM) model obtains an RMSE value of 67 um. Within the spectrum of drop widths in our dataset, ranging from 1.6 mm to 4.4 mm, this RMSE indicates that with our approach we can predict the width of sliding drops with an error of 2.4%.

AKPIK 3.3 Thu 11:00 Poster B

Performance comparison of heteroscedastic and homoscedastic noise models in Bayesian optimization — •Tatu Linnala[1], Armi Tiihonen[1], Matthias Stosiek[1], Milica Todorović[2], and Patrick Rinke[1] — [1]Department of Applied Physics, Aalto University, FI-00076, Aalto, Finland — [2]Department of Mechanical and Materials Engineering, University of Turku, FI-20014, Turku, Finland

Bayesian optimization (BO) is a machine learning method for global optimization of black-box functions. It is increasingly being used in computational and experimental optimization tasks, such as optimizing materials structure, composition, and processing conditions for targeted applications. A common assumption in BO is that noise has a uniform variance across the optimization space (homoscedastic). In experimental measurements, however, the noise variance depends on, for example, the location in the optimization space (heteroscedastic). We implemented heteroscedastic noise models in the Bayesian Optimization Structure Search (BOSS) code. We benchmarked heteroscedastic BO against homoscedastic BO with 10 different 1- to 3-dimensional noisy target functions using Gaussian process regression surrogate models. Two distinct types of heteroscedastic noise were used: in one, the noise depended on the absolute value of the target function, and in the second, on the location in the optimization space. Heteroscedastic models converge with considerably fewer BO iterations than homoscedastic ones with 9 out of the 10 investigated target functions. Thus, heteroscedastic surrogate models should be considered for experimental cases with heteroscedastic noise behaviour.

AKPIK 3.4 Thu 11:00 Poster B

Prospects of hybrid atomic-photonic neural networks for neuromorphic computing — •Mingwei Yang[1,2], Elizabeth Robertson[1,2], Kilian Junicke[2], Lina Jaurigue[3], Kathy Lüdge[3], and Janik Wolters[1,2] — [1]Deutsches Zentrum für Luft- und Raumfahrt, Institute of Optical Sensor Systems, Berlin, Germany. — [2]Technische Universität Berlin, Berlin, Germany. — [3]Technische Universität Ilmenau, Institute of Physics, Ilmenau, Germany

Optical neural networks have been identified as promising for neuromorphic computer hardware, attributed to their inherent parallelism, fast processing speeds, and low energy consumption. We discuss how photonic networks can be combined with atomic vapors providing optical non-linearities and memory functionality. In particular, we discuss an implementation of a convolutional neural network with a saturable absorber for optical nonlinearity [1], a reservoir computing architecture with atomic memory [2], and the prospects of such systems as the Ising model solver.

[1] Yang, Mingwei, et al. "Optical convolutional neural network with atomic nonlinearity." Optics Express 31.10 (2023): 16451-16459.

[2] Jaurigue, Lina, et al. "Reservoir computing with delayed input for fast and easy optimisation." Entropy 23.12 (2021): 1560.

AKPIK 3.5 Thu 11:00 Poster B

Optical data processing for machine learning on board of satellites — •Inna Kviatkovsky[1,2], Okan Akyüz[1,2], Elizabeth Robertson[1,2], Mingwei Yang[1,2], Felix Kübler[2], José Diez López[2], Enrico Stoll[2], and Janik Wolter[1,2] — [1]Deutsches Zentrum für Luft- und Raumfahrt, Institute of Optical Sensor Systems, Berlin, Germany. — [2]Technische Universität Berlin, Berlin, Germany

Resurgent interest in neural networks for machine learning renewed the excitement in the field of optical computers, seeking alternatives to the high resource intensive electronic processors. The high energy efficiency of optical vector-matrix multiplication suggests a significant energy advantage for optical processors. Such power efficiency is particularly valuable when dealing with a limited energy budget, when facing machine learning tasks in space. One obstacle for the implementations of optical compute systems is the digital-optical domain crossing, hampering both the speed and power efficiency of the computation. In this work, we target the digital to analog speed bottleneck via a 10 GHz digital to analog conversion for 4 input channels in parallel. For the compute modules free space and integrated approaches are investigated, harnessing the advantages of each. In this contribution we focus on the free space implementation, the input light from the 4 channels is shaped and interfaced with a two-dimensional intensity profile via a spatial light modulator to form a vector-matrix operation. This demonstration serves as proof of principle for further integration of optical compute modules in orbit.

AKPIK 3.6 Thu 11:00 Poster B

Unraveling Chronic Disease Relationships: A Comparative Analysis of Clustering Algorithms on the DHS 2019-2021 Indian Dataset — •Jannis Demel, Anna Nitschke, Carlos Brandl, Jonathan Berthold, and Matthias Weidemüller — Physikalisches Institut, Ruprecht-Karls Universität Heidelberg, Im Neuenheimer Feld 226, 69120 Heidelberg, Germany

Clustering algorithms play a pivotal role in unsupervised machine learning, offering a systematic approach to discerning patterns and associations within intricate datasets. The focus of application is the DHS 2019-2021 dataset from India, utilizing biomarkers to identify clusters of individuals. We compare four distinct clustering algorithms (K-means, DBSCAN, GMM, and HDBSCAN) and evaluate their performances from a data analytics and medical point of view. This approach aims to unveil novel insights into the relationships between chronic diseases. Through this poster, we contribute to a nuanced understanding of chronic diseases in India, offering valuable insights into the practicality of clustering algorithms in healthcare analytics.

AKPIK 3.7 Thu 11:00 Poster B

Phase retrieval by a conditional Wavelet Flow: applications to near-field X-ray holography — •Ritz Aguilar[1], Yunfan Zhang[1], Anna Willmann[1], Erik Thiessenhusen[1], Johannes Dora[2], Johannes Hagemann[2], Andre Lopes[3], Imke Greving[3], Berit Zeller-Plumhoff[3], Markus Osenberg[4], Michael Bussmann[1], and Jeffrey Kelling[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany — [2]Deutsches Elektronen-Synchrotron, Hamburg, Germany — [3]Helmholtz-Zentrum Hereon, Geesthacht, Germany — [4]Helmholtz-Zentrum Berlin, Berlin, Germany

Phase retrieval (PR) is an ill-posed inverse problem with several applications in medical imaging and materials science. Conventional PR algorithms either simplify the problem by assuming certain object properties and optical propagation regimes or tuning a large number of free parameters which is a time-consuming process. To circumvent this, a machine learning algorithm based on normalising flows (NF) can be used for good inversion, efficient sampling, and fast density estimation of complex-valued distributions. Here, complex wavefield data are trained on a NF-based model called conditional Wavelet Flow (cWF) which adds a conditioning network on top of the Wavelet Flow algorithm. It directly models the conditional data distribution of high resolution images and takes advantage of the parallelized training of different image resolutions, allowing for faster training of large datasets. The trained cWF is then applied to near-field X-ray holography data wherein fast and high-quality image reconstruction is made possible.

AKPIK 3.8 Thu 11:00 Poster B

Coupling experiment and simulation through a digital infrastructure for materials science — •Marian Bruns[1], Jan Janssen[1], Tilmann Hickel[1,2], and Jörg Neugebauer[1] — [1]Max-Planck-Institut für Eisenforschung GmbH — [2]Bundesanstalt für Materialforschung und -prüfung

Continuum-scale simulations require materials-parameters as input, either obtained in experiments or calculated from first principles. This process might require cumbersome, manual adjustments, especially for hardly accessible data. Also, a lack of established frameworks for sharing multiscale data hampers collaborations. This includes shortcomings in the semantic documentation of data acquisition and workflows lacking reproducibility. A major goal of the initiative "Platform MaterialDigital" is to address these issues via a prototypical infrastructure. Participants can access and set up digital environments providing tools for different steps of the scientific workflow. Data pre- and post-processing can be performed as well as simulations via the integrated development environment pyiron. We show the advantages of the interplay of digital infrastructure, ontologies, and workflows in a digital framework. Mechanical properties of a S355 steel grade are evaluated. Initially, we perform data exploration, acquisition and processing by using the semantic description of metadata hosted on a remote triplestore, enabling us to calculate elastic moduli after cold rolling. This information is used as an input for a continuum-scale simulation on uniaxial compression. We demonstrate how the different steps can be performed via a web-based interface on a provided infrastructure.

AKPIK 3.9 Thu 11:00 Poster B

Extrapolating tipping points and simulating non-stationary dynamics of complex systems using efficient machine learning — •Daniel Köglmayr and Christoph Räth — DLR KI-Sicherheit Ulm Deutschland

Model-free and data-driven prediction of tipping point transitions in nonlinear dynamical systems is a challenging and outstanding task in complex systems science. We propose a novel, fully data-driven machine learning algorithm based on next-generation reservoir computing to extrapolate the bifurcation behavior of nonlinear dynamical systems using stationary training data samples. We show that this method can extrapolate tipping point transitions. Furthermore, it is demonstrated that the trained next-generation reservoir computing architecture can be used to predict non-stationary dynamics with time-varying bifurcation parameters. In doing so, post-tipping point dynamics of unseen parameter regions can be simulated.