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 inplane 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.