AKPIK 3: AKPIK Postersession

Time: Thursday 13:30–15:30 Location: P

AKPIK 3.1 Thu 13:30 P

Towards optical neuromorphic hardware at Cesium wavelength — •Elizabeth Robertson[1,2], Mingwei Yang[1], Luisa Esguerra[1], Leon Messner[1], Lina Jaurigue[2], Guillermo Gallego[2,3], Kathy Lüdge[2], and Janik Wolters[1,2,3] — [1]Deutsches Zentrum für Luft- und Raumfahrt, Institute for Optical Sensor Systems, Rutherfordstraße 2, 12489 Berlin, Germany — [2]Technische Universität Berlin, Str. des 17. Junis 135, 10623 Berlin, Germany — [3]Einstein Center Digital Future Robert-Koch-Forum, Wilhelmstraße 67, 10117 Berlin, Germany

With the exponential growth of research in Machine Learning, so too has the demand for fast, energy efficient neuromorphic hardware, to execute such algorithms. Optics provides an attractive tool for implementing neuromorphic hardware due to is speed, low crosstalk and high parallelism. In particular, convolutional- and recurrent neural networks benefit from an optics implementation; by using passive optics to carry out convolution [1], and time division multiplexing to demonstrate a reservoir computer [2]. We present our results towards realizing an optical convolutional neural network with an atomic nonlinearity [3] and an all-optical reservoir computer based on a delay loop with an additional optical random-access memory (RAM)[4].

[1] Miscuglio, M. et al. Optica 7, 1812-1819 (2020).
[2] Brunner, D., et al. Nat Commun 4, 1364 (2013).
[3] Yang, M. et al. CLEO/Europe-EQEC, poster JSIV-P.4 (2021).
[4] Wolters, J., et al. Phys. Rev. Lett. 119, 060502 (2017).

AKPIK 3.2 Thu 13:30 P

Optical Convolutional Neural Network with Atomic Non linearity — •Mingwei Yang[1,2], Elizabeth Robertson[2,3], Luisa Esguerra[2,3], and Janik Wolters[2,3] — [1]Humboldt Universität zu Berlin, Newtonstr.15, D 12489 Berlin, Germany — [2]Deutsches Zentrum für Luft und Raumfahrt e.V. (DLR), Rutherfordstraße 2, D 12489, Berlin, Germany — [3]Technische Universität Berlin, Straße des 17. Juni 135, D 10623, Berlin, Germany

An optical convolutional neural network is demonstrated in which linear operations are implemented by lenses and spatial light modulators (SLMs), while an optical nonlinearity is realized by a cesium vapor cell as a saturable absorber. We use this network to demonstrate nonlinear image processing, as well as to improve the classification of the MNIST data by a single layer fully connected.

AKPIK 3.3 Thu 13:30 P

Convolutional Neural Network Framework for the Analysis of X-ray photoelectron spectra — •Lukas Pielsticker[1], Rachel L. Nicholls[1], Gudrun Klihm[1], Robert Schlögl[1,2], and Mark Greiner[1] — [1]Department Heterogeneous Reactions, Max Planck Institute for Chemical Energy Conversion, Mülheim an der Ruhr — [2]Department Inorganic Chemistry, Fritz Haber Institute of the Max Planck Society, Berlin

X-ray photoelectron spectroscopy (XPS) enables studying the electronic structure and chemical state of solid materials and their surfaces. Quantitative analysis of the phases present in XP spectra is typically performed by manual peak fitting. However, such elemental quantification often suffers from, among other things, superposition of core-levels of different elements, incorrect instrument calibration, poor choice of backgrounds and lineshapes, as well as from noise in the data. Moreover, as XPS instruments are becoming increasingly automated and capable of producing large amounts of data, an equally automated approach to elemental quantification is desirable.

Here, a scalable automation framework for XPS analysis using Convolutional Neural Networks (CNNs) is presented. For model training, synthetic mixed metal-oxide spectra were generated based on known reference spectra. CNNs are shown to be capable of quantitatively determining the presence of metallic and oxide phases, as well as identifying morphological features such as over- and sublayers, exhibiting more reliable performance than standard XPS users. The use of Bayesian CNNs for the determination of quantification uncertainty is illustrated.

AKPIK 3.4 Thu 13:30 P

Conversion of Molecular Dynamics (MD) simulations to Neutronand X-Ray Scattering Data using High Performance Computing — •Arnab Majumdar[1], Sebastian Busch[1], and Martin Müller[2] — [1]Lichtenberg Strasße 1, 85747, Garching b. München — [2]Leibnitz Straße 19, 24098, Kiel

Sassena is one of the software solutions to convert molecular dynamics (MD) simulations into elastic and quasi-/inelastic neutron and X-ray scattering curves. Current work makes an effort to introduce different strategies of parallel computing into sassena. Parallel computing can be a huge leap in the journey of reducing the computing time within sassena. It consists of different strategies like distributed memory parallelization(MPI), shared memory parallelization (OpenMP) and vectorization. Sassena inherits distributed memory parallelization from its previous version. This work further augments vectorization and shared memory parallelization into it. Through vectorization, this work bolsters the computing speed of sassena to a new height of up to an order of magnitude faster than its previous version. On the other hand, shared memory parallelization introduces a possibility of doing hybrid parallelization within sassena. Furthermore, this work plans to benefit from the achieved performance gain by validating simulations of hydrogen storage materials with neutron scattering data.

AKPIK 3.5 Thu 13:30 P

Making computation material science data FAIR — •Jens Bröder[1,2], Volker Hofmann[1,2], Daniel Wortmann[3], Stefan Blügel[3], and Stefan Sandfeld[1,2] — [1]Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany — [2]Helmholtz Metadata Collaboration, Hub Information — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

For research data to be reusable by scientists or machines, the gathered research data and metadata should comply with the so-called "FAIR principles", i.e. it should be findable, accessible, interoperable, and reusable [1], a task which is not straightforward. In computational materials science, workflows often encompass many different simulation steps. The enrichment of data with detailed metadata is often only feasible close to the data creation process. Therefore, designated software, workflows, tools and standards will be needed throughout the community. Using an exemplary research project, we show in detail how to reconcile data from simulations with FAIR principles. The project contains data from a high-throughput simulation performed with the program FLEUR (www.flapw.de) using the AiiDA framework (https://aiida.net) on over 5000 different materials. All data and software is openly available and FAIR through the materialscloud archive [2]. We also discuss challenges for the domain of material science and how the Helmholtz Metadata Collaboration (HMC) tries to address these issues. [1] Wilkinson, M.D.et al. Sci Data 3, 160018 (2016) [2] L. Talirz et al., Sci Data 7, 299 (2020)

AKPIK 3.6 Thu 13:30 P

Design and validation of a Digital Twin for prostate cancer from a physics point of view — •Carlos Andres Brandl[1], Anna Nitschke[1], and Matthias Weidemüller[1,2] — [1]Physikalisches Institut, Ruprecht-Karls Universität Heidelberg, Im Neuenheimer Feld 226, 69120 Heidelberg, Germany — [2]National Laboratory for Physical Sciences at Microscale and Department of Modern Physics, and CAS Center for Excellence and Synergetic Innovation Center in Quantum Information and Quantum Physics, Shanghai Branch, University of Science and Technology of China, Shanghai 201315, China

Digital Twins (DT) are virtual representations of physical assets and e.g. promise improved decision making. DT can help to personalize healthcare for complex diseases like prostate cancer by combining large amount of clinical parameters and answering the questions of tumor risk, tumor stage and optimal treatment. In medical applications interpretability and uncertainty quantification are crucial.

Combining data-driven approaches with interpretable machine-learning models and evidence based clinical guidelines will lead to more reliable and confidential outcomes. Correlation analysis gives an insight to the data and enables to unravel the dependencies of important clinical parameters like prostate specific antigen (PSA) with others and determine their distributions in the Heidelberg patient cohort. The backpropagation of outcome errors to the found distributions of the input parameters with Bayesian methods allows to determine the impact of the input parameter uncertainties on the twin predictions and helps clinicians to interpret the results accordingly.

AKPIK 3.7 Thu 13:30 P

Comparison of structural representations for machine learning-accelerated *ab initio* calculations — •Johannes Wasmer, Philipp Rüssmann, and Stefan Blügel — Forschungszentrum Jülich, Germany

Quantum mechanical calculations based on density functional theory (DFT) are the workhorse in today's computational materials design. Here we explore the possibility to accelerate the DFT calculations with potentials generated from a surrogate machine learning model. Finding a better starting potential could drastically reduce the number of required self-consistency steps during the convergence of DFT calculations. The juKKR code (jukkr.fz-juelich.de) allows high-throughput *ab initio* impurity embedding calculations which we use to generate a training dataset of 10'000 impurities from most elements of the periodic table embedded into elemental crystals with the help of the workflow engine AiiDA. The choice of a structural representation of the atomic environment which a machine learning model can understand has been identified as a crucial step. We compare a variety of such representations as training input for our surrogate model. Finally, we benchmark results for the converged impurity potential from DFT calculations against the output of the trained surrogate model.

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