AKPIK 6: AI Methods for Physics and Materials Science

Time: Thursday 16:45–18:30 Location: BEY/0127

AKPIK 6.1 Thu 16:45 BEY/0127

Recycling resources from aborted quantum key distribution protocols — •Siyuan Qi[1] and Ramona Wolf[2] — [1]Universität Siegen, Siegen, Germany — [2]Universität Siegen, Siegen, Germany

In quantum key distribution protocols, abortion often occurs due to detected errors or leakages. A secure protocol must ensure that if abortion does not occur, the generated key is secure. However, when abortion happens, the resources used are lost and cannot be reused, leading to waste. A malicious party, Eve, can exploit this by intentionally interfering with the protocol, forcing an abortion every time it's run. While Eve cannot obtain the secret key or avoid detection, she can prevent key generation and cause significant resource waste, which is undesirable in practical scenarios. This issue can be addressed by implementing procedures that recycle resources from aborted protocols or by preventing Eve from interfering in such a way. A protocol is aborted when the minimum entropy of the key generated does not exceed the leakage. If an abortion is caused by large leakage, we can still generate certified private randomness from the minimum entropy, provided it is not zero. Additionally, in specific scenarios where there is an identity designation process involved, we can move the identity designation to the last round so that Eve, not knowing she is a participant or not until the very end, will be discouraged from malicious behaviors.

AKPIK 6.2 Thu 17:00 BEY/0127

Causal–Physical Descriptor Discovery for Interpretable Materials Informatics — •Kanchan Sarkar and Axel Gross — Institute of Theoretical Chemistry, Ulm University, 89069 Ulm, Germany

Linking data-driven models to physically grounded behavior remains a key challenge in materials informatics. Data Nexus Vista (DNV1) is a causally informed framework that integrates domain knowledge with machine learning to identify interpretable descriptors. It provides standardized, configurable workflows spanning data preprocessing, feature construction, model training, and interpretation. DNV1 combines established feature-importance and descriptor-design tools with causal analyses, including counterfactual interventions, allowing for direct assessment of how model predictions respond to controlled changes. The framework supports both graphical and programmatic interfaces and provides descriptor-tracing utilities that map model features to physically meaningful variables. All workflows and outputs adhere to FAIR principles, ensuring reproducibility and transparency. The framework has been tested on multiple datasets and demonstrated with DFT-computed spinel cathodes. Rather than limiting ML models with fixed descriptors, DNV1 allows descriptors to emerge through causal interrogation of the data-physics nexus.

AKPIK 6.3 Thu 17:15 BEY/0127

Support for self-driving labs within the NOMAD ecosystem — •Sarthak Kapoor[1], Hampus Näsström[1], Ahmed Ilyas[1], Alvin N. Ladines[1], Alexander Fuchs[2], Joseph F. Rudzinski[1], Lauri Himanen[1], Sebastian Brückner[1], José A. Márquez[1], Martin Albrecht[3], and FAIRmat Team[1] — [1]Physics Department and CSMB, Humboldt-Universität zu Berlin, Germany — [2]Department Physik, FAU Erlangen-Nürnberg — [3]Department Materials Science, IKZ Berlin

Self-driving laboratories (SDLs) rely on robust digitization, structuring, and analysis of experimental data. We present NOMAD [nomad-lab.eu] [1] as a comprehensive research data management and workflow ecosystem that addresses the challenges inherent to emerging SDLs. The NOMAD ecosystem supports direct interfacing with lab instruments and addresses the transformation of instrument outputs into machine-actionable formats, a key requirement in SDLs, through a flexible schema system that allows researchers to represent raw data as standardized entries based on community-developed or laboratory-specific definitions. NOMAD Actions provide a robust framework for defining, executing, and monitoring sophisticated analysis and decision-making SDL workflows, such as ML pipelines and Bayesian optimization strategies. Moreover, NOMAD's workflow storage framework facilitates detailed provenance tracking, along with tools for navigating workflow graphs. Together, these capabilities position NOMAD as a foundational toolkit for realizing scalable, reliable, and FAIR SDLs. [1] Scheidgen, M. et al., JOSS 8, 5388 (2023).

AKPIK 6.4 Thu 17:30 BEY/0127

Probabilistic greedy algorithm solver using magnetic tunneling junctions for traveling salesman problem — •Ran Zhang[1,2,3], Xiaohan Li[2], Caihua Wan[2,3,4], Raik Hoffmann[5], Meike Hindenberg[5], Yingqian Xu[2], Shiqiang Liu[2], Dehao Kong[2], Shilong Xiong[2], Shikun He[6], Alptekin Vardar[5], Qiang Dai[6], Junlu Gong[6], Yihui Sun[6], Zejie Zheng[6], Thomas Kämpfe[5,7], Guoqiang Yu[2,3,4], and Xiufeng Han[2,3,4] — [1]Present address: Max Planck Institute of Microstructure Physics, Halle (Saale), Germany — [2]Institute of Physics, Chinese Academy of Sciences, Beijing, China — [3]University of Chinese Academy of Sciences, Beijing, China — [4]Songshan Lake Materials Laboratory, Dongguan, China — [5]Fraunhofer IPMS, Dresden, Germany — [6]Zhejiang Hikstor Technology Co. Ltd, Hangzhou, China — [7]TU Braunschweig, Braunschweig, Germany

Combinatorial optimization is central to AI, logistics, and network design, yet classical methods often trade efficiency for solution quality. We introduce a probabilistic greedy solver that integrates spin-transfer-torque MTJ true random number generators with tunable switching statistics. A temperature parameter controls the balance between deterministic and stochastic choices. Applied to the traveling salesman problem, the framework achieves high-quality tours and surpasses simulated annealing and genetic algorithms in convergence speed, scalability, and computational cost.

AKPIK 6.5 Thu 17:45 BEY/0127

FAIR and Flexible Workflow Support within the NOMAD Infrastructure — •J.F. Rudzinski[1], T. Bereau[2], S. Botti[3], E.B. Boydas[1], N. Daelman[1], L. Himanen[1], S. Kapoor[1], A.N. Ladines[1], J.A. Márquez[1], B. Mohr[1], H. Näsström[1], and Fairmat Team[1] — [1]CSMB, HU Berlin — [2]ITP, Heidelberg Uni. — [3]RC-FEMS, Ruhr Uni. Bochum

NOMAD [nomad-lab.eu] [1, 2] is an open-source, community-driven research data infrastructure designed for modern physics. It provides FAIR-compliant storage, management, and analysis for diverse computational and experimental materials science data, and its modular, plugin-based architecture enables low-barrier extensions for adjacent and interdisciplinary domains. Here we present NOMAD*s workflow capabilities as a foundation for scalable and AI-ready data pipelines. A general workflow schema supports both standardized and custom workflows that record detailed provenance and link heterogeneous data streams. Standardized workflows enable powerful search, visualization, and automation features, while custom workflows support agile, project-specific digitalization. Workflow entries can be created via Python-based plugins, a YAML workflow specification, or the NOMAD ELN interface, ensuring accessibility for researchers with varying technical backgrounds. Combined with a toolkit for high-throughput interfacing, NOMAD provides a robust and sustainable digital infrastructure across physics subdisciplines.

[1] Scheidgen, M. *et al.*, JOSS **8**, 5388 (2023).
[2] Scheffler, M. *et al.*, Nature **604**, 635-642 (2022).

AKPIK 6.6 Thu 18:00 BEY/0127

Towards machine-learning-based on-the-fly analysis of neutron reflectometry — •Anne Rentzsch[1], Valentin Munteanu[1], Oliver Anyanor[2], Shreya Shah[1], Philipp Gutfreund[3], Rémi Perenon[3], Anthony Higgins[2], Vladimir Starostin[4], Alexander Hinderhofer[1], Dmitry Lapkin[1], and Frank Schreiber[1] — [1]Institut für Angewandte Physik, Universität Tübingen, 720726 Tügingen — [2]School of Engineering and Applied Science, Swansea University, Swansea SA1 8EN, Wales, United Kingdom — [3]Institut Laue-Langevin, 38000 Grenoble, France — [4]Cluster of Excellence 'Machine learning - new perspectives for science', Universität Tübingen, Maria-von-Linden-Straße 6, 72076 Tübingen, Germany

We present a real-time data analysis pipeline for neutron reflectometry that integrates `reflectorch`, a machine-learning-based software for reflectometry data analysis, into the IT infrastructure at the Institut Laue-Langevin. The workflow was tested during an experiment on the mixing behavior of bilayer thin films. Measured data are automatically reduced and analyzed, and the predicted sample parameters are returned to the instrument control system. The automated analysis can be triggered as frequently as every 10 seconds, enabling parameters

and their uncertainties to be tracked with high temporal resolution and supporting continuous monitoring and data-driven adjustments. Compared to conventional software, `reflectorch` is up to two orders of magnitude faster. Together, these results pave the way for closed-loop experiments and demonstrate the potential of machine learning to enhance the efficiency of neutron reflectometry experiments.

AKPIK 6.7 Thu 18:15 BEY/0127

Multi-fidelity and -objective optimization of ONCV pseudopotentials — •Austin Zadoks[1], Cameron Hargreaves[2], Jusong Yu[1], Weiguo Jing[2], Matteo Giantomassi[2], Gian-Marco Rignanese[2], and Giovanni Pizzi[1] — [1]PSI Center for Scientific Computing, Theory and Data, 5232 Villigen PSI, Switzerland — [2]Institute of Condensed Matter and Nanosciences, UCLouvain, Louvain-la-Neuve, Belgium

The pseudopotential (PSP) approximation is essential to the tractability of many first-principles methods. However, it requires balancing the number of pseudized states, basis-set convergence, and accuracy w.r.t. all-electron (AE) results. One notable method for constructing soft, faithful, and widely-supported PSPs is the optimized norm-conserving Vanderbilt (ONCV) approach[1]. Various strategies have been proposed for generating meta-optimal tables of ONCVPSPs such as the SG-15[2], PseudoDojo[3], and SPMS[4]. Recent efforts to verify DFT codes have highlighted the importance of high-quality PSPs and expanded the necessary AE reference data, notably through $Z = 96$[5]. We present a fully-automated multi-fidelity multi-objective Bayesian optimization of ONCVPSPs targeting these reference data. This approach allows for the efficient mapping of the high-fidelity PW-DFT Pareto frontier by leveraging lower-fidelity intermediate radial- and PW-DFT results.
[1]D.R. Hamann. PRB, 88 (2013). [2]M. Schlipf & F. Gygi. Comp. Phys. Comms., 196 (2015). [3]M.J. van Setten, et al. Comp. Phys. Comms., 226 (2018). [4]M.F. Shojaei, et al. Comp. Phys. Comms., 283 (2023). [5] E. Bosoni, et al. Nat. Rev. Phys., 6 (2024).