AKPIK 3: Research with AI: Hardware, Software, Tools

Time: Tuesday 11:00–12:45 Location: BEY/0127

AKPIK 3.1 Tue 11:00 BEY/0127

Agentic Exploration of Physics Models — •Maximilian Nägele[1,2] and Florian Marquardt[1,2] — [1]Max Planck Institute for the Science of Light — [2]FAU Erlangen

The process of scientific discovery relies on an interplay of observations, analysis, and hypothesis generation. Machine learning is increasingly being adopted to address individual aspects of this process. However, it remains an open challenge to fully automate the heuristic, iterative loop required to discover the laws of an unknown system by exploring it through experiments and analysis, without tailoring the approach to the specifics of a given task. Here, we introduce SciExplorer, an agent that leverages large language model tool-use capabilities to enable exploration of systems without any domain-specific blueprints, and apply it to physical systems that are initially unknown to the agent. We test SciExplorer on a broad set of models spanning mechanical dynamical systems, wave evolution, and quantum many-body physics. Despite using a minimal set of tools, primarily based on code execution, we observe impressive performance on tasks such as recovering equations of motion from observed dynamics and inferring Hamiltonians from expectation values. The demonstrated effectiveness of this setup opens the door towards similar scientific exploration in other domains, without the need for finetuning or task-specific instructions.

AKPIK 3.2 Tue 11:15 BEY/0127

Executable Manuscripts as Jupyter Notebooks: The Next Evolution in Scientific Publishing? — •Sebastian Rejman[1,2], Ina Vollmer[2], and Bert Marc Weckhuysen[2] — [1]Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany — [2]Utrecht University, Utrecht, The Netherlands

The scientific paper as we know it today has remained largely unchanged for over a century. While color figures are now standard, and the supporting information contains more and more of the evidence, the manuscript itself remains a static pdf. The tools available to us, however, have drastically improved. Internet connections are faster, compute and storage are cheap, and high-level programming languages like Python make analysis automation accessible to the non-expert programmer.

Jupyter Notebooks, familiar to many students learning to program, allow to combine text with code and interactive figures. These notebooks, if used together with data repositories like OSF along with analysis code hosted on GitHub, allow for a transparent and reusable publication of research results. The reader can reproduce the analysis and figures at the push of the button, and easily re-purpose both analysis code and the underlying data - Paving the way for studies with large datasets in the field of chemistry and the natural sciences in general.

In this contribution, we demonstrate the executable version of our recent work on the role of external acidity in the cracking of plastics and provide practical guidance for implementation.

AKPIK 3.3 Tue 11:30 BEY/0127

PaperVerse: Disrupting the Peer-Review Process via AI-Driven Analysis and Reviewer Compensation — •Hendik Zobel, Oliver Mey, and René Stemmler — PaperVerse UG (haftungsbeschränkt), Dresden, Germany

The current scientific publishing model faces a systemic bottleneck: it relies on the uncompensated labor of volunteer researchers, resulting in significant delays and undervalued expertise. This talk introduces PaperVerse, a platform designed to disrupt this paradigm by treating peer review as valuable, billable work - supported by generative AI.

We propose a dual-layer architecture. First, our active AI Review Engine provides immediate, automated feedback on preprints (e.g., from arXiv) and private uploads, allowing authors to iteratively improve their manuscripts before submission. Second, and most critically, we outline our vision for a monetized marketplace that directly compensates human reviewers. By offloading structural and stylistic critique to AI, we free experts to focus on deep scientific validation, ensuring they are financially rewarded for their intellectual contribution.

We will discuss how AI-driven insights pave the way for this shift from volunteerism to a fair, incentivized economy. PaperVerse aims to establish a sustainable ecosystem where algorithmic efficiency meets human expertise, finally giving peer review the market value it deserves.

Invited Talk AKPIK 3.4 Tue 11:45 BEY/0127

Model-free training of optical neural networks based on multimode semiconductor lasers — •Anas Skalli[1], Satoshi Sunada[2], Mirko Goldmann[1], Marcin Gebski[3], Nasibeh Haghighi[4], Stephan Reitzenstein[4], James A. Lott[4], Tomasz Czyszanowski[3], and Daniel Brunner[1] — [1]FEMTO-ST Institute / Optics Department, CNRS & Université Marie et Louis Pasteur, 15B avenue des Montboucons, 25030 Besançon Cedex, France. — [2]Faculty of Mechanical Engineering, Institute of Science and Engineering, Kanazawa University, Kakuma-machi Kanazawa, Ishikawa 920 1192, Japan. — [3]nstitute of Physics, Lodz University of technology, Wólczańska 217/22190-005 Łódź, Poland — [4]Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstraße 36, 10623 Berlin, Germany

In this work, we demonstrate a fully autonomous and parallel optical neural network (ONN) based on a multimode VCSEL architecture using off-the-shelf components. The system is scalable in both network size and inference bandwidth, paving the way toward GHz-level computing. Our ONN supports in-situ learning, making it closer to true autonomous operation. To unlock the full potential of our hardware, we develop and benchmark several hardware-compatible optimization algorithms, including SPSA and PEPG, demonstrating their suitability for physical systems with limited computational resources, and showing how algorithmic choices impact convergence speed, scalability, and energy cost. Our ONN outperforms both a linear hardware baseline and a digital linear classifier on the MNIST task.

Invited Talk AKPIK 3.5 Tue 12:15 BEY/0127

Virtual Reality Gamification for Photonics, AI and More — •Arash Rahimi-Iman — I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

Amazing mixed or virtual reality (XR/VR) tools can boost excitement for various science topics across age groups. VR-enhanced lectures can visually address topics such as photonics or artificial intelligence, illustrate what space travel or a visit to periodic lattices of solids might be like, allow learners to play with beams and particles to solve quests, and do much more.

Game-like exploration environments can support self-paced learning and collaborative training, including multiplayer modes. This not only brings immersion, but also interaction and fun. Moreover, VR worlds can help circumvent typical limitations of traditional labs, such as access, safety, or resources. They promote an extraordinary variety of designs and implementations, such as toy experiments mimicking, for instance, laser optics, quantum and nanophysics, and more.

Here, I present in VR one example of a digital learning environment enabled by powerful computer game engines like UE5. Like a lab-on-a-chip combining several laboratory functions on a single integrated circuit, hence on a chip, my VR analog "lab-in-a-chip" (the virtual lab world) could bring together different virtual experiments and learning scenarios, with user-group–oriented gamification making them more tangible for learners and non-experts.