AKPIK 5: Poster

Time: Thursday 15:00–16:30 Location: P2

AKPIK 5.1 Thu 15:00 P2

Photonic Matrix-Vector Multiplication at the Quantum Limit of single photons — •Mingwei Yang[1,2], Okan Akyüz[2], Felix Kübler[2], Konrad Tschernig[1], Xavi Barcons[1,3], Enrico Stoll[2], 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]Humboldt-Universität zu Berlin, Berlin, Germany.

Photonic integrated circuits (PICs) have emerged as a promising solution for performing energy-efficient matrix multiplication and addition operations (MACs) in neural networks [1]. In this work, we demonstrate a 4x4 optical matrix-vector multiplication (MVM) using a mesh of Mach-Zehnder interferometers (MZIs), operating with attenuated laser pulses at the single-photon level. Using this as an example, we analyze the quantum limit of energy consumption of optical systems for classical machine learning. [1] Wetzstein, Gordon, et al. "Inference in artificial intelligence with deep optics and photonics." Nature 588.7836 (2020): 39-47.

AKPIK 5.2 Thu 15:00 P2

Machine Learning Optimization of Chiral Photonic Nanostructures — •Davide Filippozzi[1], Nicolas Roy[2], Alexandre Mayer[2], and Arash Rahimi-Iman[1] — [1]I. Physikalisches Institut and Center for Materials Research, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany — [2]NaXys, Namur Institute for Complex Systems, University of Namur, Belgium

Deep learning (DL) and evolutionary algorithms (EA) as part of the machine learning (ML) domain have recently been well utilized for optimization purposes, such as for nanostructure design. Particularly, unintuitive problems can benefit from the potential abstraction levels that artificial Neural Networks (NNs) can achieve based on sufficient training and proper data. Reinforcement learning approaches promise to boost inference of solutions for complicated design requirements and specific functionalities.

We present a study that discusses the nano-pattern design optimization with a combination of DL and EA for a dielectric surface's preference for single-handed circularly polarized light in reflection or transmission. Advancing our previous simulations and algorithms [O. Mey and A. Rahimi-Iman, Phys. Status Solidi RRL 2022, 16, 2100571], the optimization in chiral dichroism and reflectivity for our metasurface's design is discussed. Such ML optimization can improve desirable features of unintuitive metamaterials and photonic nanostructures, as increasingly highlighted in up-to-date literature.

AKPIK 5.3 Thu 15:00 P2

Towards an ontology-based digital twin for graphene-based conductor materials — •Fabian Teichert[1,2,3], Leonhard Niemann[4,5], Florian Fuchs[1,2,3], Jörg Schuster[1,2,3], and Martin Köhne[4] — [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]Department of Advanced Technologies and Micro Systems, Robert Bosch GmbH, Renningen, Germany — [5]Faculty of Natural Sciences, Chemnitz University of Technology, Chemnitz, Germany

The „Platform Material Digital" (www.materialdigital.de) advances digital twins within material science, based on a semantic description using ontologies. The aim is to digitally represent (new) materials, their properties and crucial processing steps. We are actively involved in this endeavour by digitalizing graphene-based conductor materials. An ontology is created and enriched with simulation data and experimental data, covering various aspects such as model parameters, preparation processes, and measurement processes. We create the following demonstrator use cases with a semantic data description: (1) the integration of our simulation methods as workflows within the „Platform Material Digital", (2) an App to store, filter, and post-process our production and measurement processes and material properties of the graphene-based conductor materials.

AKPIK 5.4 Thu 15:00 P2

Machine learning to resolve the structure: Perovskites and related materials — •Ekaterina Kneschaurek, Vladimir Starostin, Valentin Munteanu, Constantin Völter, Damian Balaz, Mikhail Romodin, Maik Hylinski, Dmitry Lapkin, Ivan Zaluzhnyy, Alexander Hinderhofer, Alexander Gerlach, and Frank Schreiber — University of Tübingen, Tübingen, Germany

Recent advances in synthesis of novel materials used in solar cells, such as perovskites, are supported by structural analysis, using X-rays. To unravel the complexity of such materials, we utilize both *in situ* (studying crystallization kinetics) and *ex situ* (accessing phase composition) X-ray diffraction. The high-resolution scattering patterns are recorded by large 2D detectors, resulting in enormous amounts of data, which are difficult to analyze manually [1]. In some cases, there are no crystallographic information files (.cif) for the newly synthesized materials. An initial guess, based on the composition of the studied material, can estimate ranges of expected scattering signals from distinct phases. The deep learning (DL) model can detect Bragg peaks within the diffraction pattern, while the application of clustering and 2D Gaussian fitting enables the processing of complex data to be conducted more effectively. Preliminary data analysis of 2D patterns in real time can increase the efficiency of beamtimes and provide a feedback loop to optimize the parameters of the experiment.

[1] Hinderhofer, A., Greco, A., Starostin, V., Munteanu, V., Pithan, L., Gerlach, A., Schreiber, F. (2023). J. Appl. Cryst. **56**, 3-11.

AKPIK 5.5 Thu 15:00 P2

Balancing the Cart-Pole: Deep Q-Networks vs. Echo State Networks — •Igor Polonskiy, Atreya Majumdar, and Karin Everschor-Sitte — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47057 Duisburg, Germany

Balancing a pole on a moving cart by applying directional forces is a standard benchmark problem in reinforcement learning. Deep Q-Networks [1], which integrate reinforcement learning with neural networks, have been highly effective in solving this problem. However, their reliance on multiple hidden layers makes them computationally intensive and energy-demanding. Replacing these hidden layers with an Echo State Network reduces trainable parameters and energy consumption. In this study, we compare the performance of Deep Q-Networks and Echo State Networks on the Cart-Pole problem. We show that an Echo State Network-Q-Network combination, with sufficient size and runtime, can not only match but also surpass Deep Q-Networks in cumulative rewards and control success rates.

[1] V. Mnih et al., Nature 518, 529 (2015)

AKPIK 5.6 Thu 15:00 P2

Latent Measures of Memory and Stochasticity in Dynamical Systems: Murphy's Law of Tumbling Toast — •Janine Graser, Atreya Majumdar, Kübra Kalkan, Ross Knapman, and Karin Everschor-Sitte — Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of DuisburgEssen, 47057 Duisburg, Germany

Murphy's Law, which suggests that "anything that can go wrong will go wrong," is often exemplified by toast landing butter-side down. In reality, a toast falling from a table can be described by Newtonian mechanics and is bound to fall on the butter side under standard conditions [1]. Here, the fall is modelled through its seemingly hidden aspects (table height and toast asymmetry because of the butter).

We revisit the tumbling toast problem using the data-driven machine learning tools - latent entropy and latent dimension -introduced by Horenko et al. [2]. We develop a Python-based implementation that characterizes the fall using these latent measures. This approach has broader applications in other dynamical systems, such as predicting and optimizing magnetic material properties.

[1] R. A. J. Matthews, Eur. J. Phys. 16 172 (1995)
[2] I. Horenko et al., Commun. Appl. Math. Comput. Sci. 16 267-297 (2021).

AKPIK 5.7 Thu 15:00 P2

Measurement of thermal conductivity and thermal diffusivity through spatial and temporal temperature gradients — •Junsheng Zhuo[2] and Stephanie Lippmann[1,2] — [1]Institute of Applied Physics, Friedrich Schiller University Jena, Jena, Thuringia, 07745, Germany — [2]Otto Schott Institute of Materials Research, Friedrich Schiller University Jena, Jena, Thuringia, 07743, Germany

To address the challenges of measuring thermal properties of metal, a new device is being developed to measure both thermal conductivity and thermal diffusivity quickly and accurately. The sample is heated directly using an electromagnetic induction furnace, avoiding thermal resistance issues. High-resolution infrared cameras capture temperature distribution with ultra-short time and space intervals, allowing for precise thermal conductivity and diffusivity measurements. Mineral oil is used for cooling, enabling rapid heat transfer. This device calculates temperature-dependent thermal conductivity using spatial temperature gradients and heat flow, based on Fourier's law assisted by fitting, statistics, and machine learning, while thermal diffusivity is derived from real-time transient temperature gradients using the inverse method. Specific heat capacity is then calculated from these two values.

AKPIK 5.8 Thu 15:00 P2

Deterministic Model of Multi-Agent Boltzmann Q-Learning: Transient Dynamics, Feedback Loops, and Non-Convergence — •David Goll[1], Jobst Heitzig[2], and Wolfram Barfuss[3] — [1]Humboldt University of Berlin — [2]Potsdam Institute of Climate Impact Research — [3]University of Bonn

Multi-Agent Reinforcement Learning involves interacting agents whose learning processes are indirectly coupled through their shared environment, giving rise to emergent, collective dynamics that are sensitive to initial conditions and parameter variations. A Complex Systems approach, which examines dynamic interactions in multi-component systems, can uncover the underlying dynamics by constructing deterministic, approximate models of stochastic algorithms. In this work, we show that even in the simplest case of independent Q-learning with a Boltzmann exploration policy, previous models fail to capture actual learning behaviour. Specifically, the dynamics of the Q-space—representing agents' state-action value estimates—cannot be directly reduced to the lower-dimensional policy space representing their strategies, as assumed in earlier models. By explicitly incorporating agents' update frequencies, we propose a new discrete-time model that captures the observed behaviours and uncovers a fundamentally more complex dynamical landscape. We demonstrate the utility of this approach by applying it to the Prisoner's Dilemma, where our model distinguishes transient states, which might be mistaken for equilibria, from true equilibria. Furthermore, we show that varying hyperparameters, such as the discount factor, can prevent convergence to a joint policy.

AKPIK 5.9 Thu 15:00 P2

Noisy quantum computing of electronic structure of crystals — •Vojtěch Vašina[1,2], Ivana Miháliková[1], and Martin Friák[1] — [1]Institute of Physics of Materials, Czech Academy of Sciences, Brno, Czech Republic — [2]Brno University of Technology, Brno, Czech Republic

Quantum computing is currently emerging as a useful paradigm for solving highly complex computational problems. Current quantum computers are unfortunately too noisy to provide sufficient accuracy, and quantum-classical hybrid algorithms emerged as a solution. Variational Quantum Eigensolver (VQE) has gained significant attention for addressing challenges in quantum chemistry, material science, etc. VQEs typically use multiple optimization methods, and the correct choice of optimization method can significantly impact performance. In our study, we focused on the comparison of multiple optimization methods used in VQE when applied to the electronic structure of crystals. The quantum part of VQE ran on a classical simulator with imported noise models from real quantum computers from the IBM Quantum Platform.

AKPIK 5.10 Thu 15:00 P2

Advancing Digital Transformation in Research on Universe and Matter in Germany — Martin Erdmann[1], •Jan M. Bürger[1], Banjamin Fischer[1], Stefan Fröse[2], Judith Steinfeld[1], and Angela Warkentin[1] — [1]RWTH Aachen University — [2]TU Dortmund University

Research on Universe and Matter (ErUM) at major infrastructures such as CERN or large observatories, jointly conducted with university groups, is an important driver for the digital transformation. In Germany, about 20,000 scientists are working on ErUM-related sciences and can benefit from actual methods of artificial intelligence. The central networking and transfer office ErUM-Data-Hub provides support by designing, organizing and performing schools and workshops for young and expert scientists in the areas of big data, machine learning, sustainable computing and many more. We present the actual achievements of the ErUM-Data-Hub in the German ErUM community.

AKPIK 5.11 Thu 15:00 P2

The graphene resonant metasurface substrate in near-zero refractive index regime to control the surface plasmon-polariton propagation length — •Zoya Eremenko — Leibniz-Institut für Festkörper- und Werkstoffforschung, Dresden, Deutschland

The study goal is to identify and investigate conditions for controlling the propagation length of graphene surface plasmon-polaritons (SPP) through the utilization of hybrid graphene-dielectric metasurfaces. We study the spectral characteristics of resonant multipole modes in all-dielectric metasurface using the photonic crystal approach, metasurface unit cell modelling approach and implement these approaches by the commercial software Comsol Multiphysics 6.2. For controlling the propagation length of graphene SPPs we used all-dielectric metasurface as a substrate of graphene layer in a near-zero refractive index regime. The determined the parameters of the near-zero refractive index regime for the studied metasurface, which is crucial for achieving the main project goal of controlling SPP propagation length in the graphene layer. Knowing the effective refractive index of the metasurface unit cell in the near-zero regime, these values are used in Comsol modeling the hybrid metasurface as a graphene layer substrate to calculate the SPP propagation length.

AKPIK 5.12 Thu 15:00 P2

Development of a Parametric Design Program for Building Construction Elements using Artificial Intelligence — •Artem Burdin — Moscow, Russia

Thesis: The aim of this research is to develop a parametric design program for building construction elements using artificial intelligence, focusing on the application of modern IT and artificial intelligence in physics-based modeling and simulation. The program will enable the creation of complex building structures, such as bridges, tunnels, and high-rise buildings, with increased accuracy and efficiency. Key objectives: * Analyze the current state of parametric design in building construction * Develop a parametric design program using artificial intelligence and machine learning algorithms * Implement the program using a suitable programming language and software * Test and validate the program using real-world examples * Evaluate the program's performance and potential applications in the construction industry Expected outcomes: * A parametric design program capable of generating complex building structures with increased accuracy and efficiency * A comprehensive analysis of the current state of parametric design in building construction * A detailed evaluation of the program's performance and potential applications in the construction industry * Contributions to the development of artificial intelligence and modern IT in physics-based modeling and simulation Keywords: parametric design, building construction, artificial intelligence, machine learning, physics-based modeling, simulation, computer-aided design (CAD), construction industry.

AKPIK 5.13 Thu 15:00 P2

Working group on physics, modern Information technologies and artificial Intelligence — •Adam Barakhoev — Moscow, Russia

Artificial intelligence and modern computer infrastructure are changing the approach to physics, combining powerful computational methods with experiments. These innovations help scientists process large amounts of data, automate complex tasks, and make accurate predictions. One of the important achievements is the use of artificial intelligence to improve physical experiments, especially in quantum mechanics and optical systems. Machine learning algorithms can predict results based on incomplete data and help set up experiments in real time, which significantly increases their efficiency and accuracy. Also, modern OT technologies, such as cloud services and high-performance computing, are important for managing the large-scale modeling needed in modern physics research.

AKPIK 5.14 Thu 15:00 P2

Autonomous Vehicles: Technologies and Challenges — •Nikita Timoshin — Moscow, Russia

Autonomous vehicles are transforming transportation with technologies such as artificial intelligence (AI), machine learning, and advanced sensor systems like LiDAR, radar, and cameras. These vehicles rely on AI to make real-time decisions, using data from various sensors through sensor fusion for accurate environmental perception. Communication networks like V2X (Vehicle-to-Everything) and 5G enable vehicles to interact with infrastructure and other vehicles.

The benefits include enhanced safety by reducing human error, improved traffic efficiency, and increased mobility for people with disabilities. However, challenges such as sensor limitations in adverse conditions, high computational demands, and ethical dilemmas about decision-making in critical situations remain. Additionally, regulatory and privacy concerns need to be addressed. As autonomous vehicles integrate with smart cities, they could significantly reshape urban mobility.

AKPIK 5.15 Thu 15:00 P2

Experimental examination of the validity of the Turing test for considering Artificial Intelligence as having subjectivity — •Lev Gelbart and Alexey Iakovlev — Moscow, Russia

The speed of development of Artificial Intelligence (AI) raises questions about its subjectivity and thinking. Alan Turing, who set the criteria for thinking, did not consider subjectivity. There are sharp discussions on this topic, for example, Doctor of Law Valery Zorkin, professor at MSU, opposes endowing AI with subjectivity, emphasising humanism.

It should also be taken into account that the Turing test may be invalid if we consider people, who are not capable of passing it. For example, a study by Alan Ropper (2010) showed that patients in a vegetative state can demonstrate brain activity, but are clearly unable to pass the Turing test, which does not detract from their human value.

We have considered, whether a machine can pass a test designed for humans. Machines are thought to not be able to adequately mimic emotions, so we tested three chatbots (Lily, AI Chat, ChatGPT) for emotional intelligence using the IDRlabs test. All chatbots performed above the average of humans (77.27%, 68.87%, 64.6%), but this, obviously, does not make them subjects of law.

Conclusion: the Turing test is not valid for assessing the subjectivity of AI.

AKPIK 5.16 Thu 15:00 P2

Unmanned transportation in the field of cargo transportation and its contribution to industry. — •Alexey Platonov — Moscow, Russia

In recent years, the transportation industry has witnessed a transformative shift towards automation and innovation, with unmanned transportation systems emerging as a pivotal force in cargo logistics.

Unmanned transportation significantly improves safety in cargo movement. By reducing the reliance on human drivers, the industry can mitigate the risks associated with human error, a leading cause of accidents in transportation.

The integration of LiDAR into cargo transportation also opens up new avenues for delivery services.

It is worth considering that the active introduction of unmanned vehicles in cargo transportation is beginning. Several test shipments of real orders were made on KamAZ-5490 trucks without direct driver control. There was only a mechanic controller in the cockpit, who checked the performance of the systems.

By enhancing efficiency, improving safety, and fostering innovation, these technologies are set to revolutionize the logistics landscape, proving that the future of transportation is indeed unmanned.

AKPIK 5.17 Thu 15:00 P2

Crawler-motor grader — •Vyacheslav Kharchevnikov — Moscow, Russia

An overview of the relevance and necessity of developing a crawler-mounted motor grader. A description of the problems that this equipment solves in the construction and road sector. An analysis of existing models of motor graders, including wheeled and tracked versions, their advantages and disadvantages. Defining the main goal of the project - to create an effective crawler-mounted motor grader. Setting the tasks necessary to achieve the goal, such as improving the cross-country ability and stability of the equipment. A detailed description of the design of a crawler-mounted motor grader, including the features of the chassis, control system and attachments.

An analysis of the economic feasibility of introducing a crawler-mounted motor grader, a comparison with traditional models, an assessment of production and operating costs. An assessment of the environmental impact of using a crawler-mounted motor grader, measures to reduce emissions and reduce noise. Summarizing the research, assessing the results achieved and prospects for further development and implementation of a crawler-mounted motor grader.

AKPIK 5.18 Thu 15:00 P2

Development of a design solution for automating a set of tasks in the production preparation subsystem of an automated control system for a small construction company — •Tikhon Shabrov — Moscow, Russia

automation of processes for small companies use of new technologies

AKPIK 5.19 Thu 15:00 P2

Acceleration of crystal structure relaxation with Deep Reinforcement Learning — •Elena Trukhan, Efim Mazhnik, and Artem R. Oganov — Moscow, Russia

We introduce a Deep Reinforcement Learning (DRL) model for the structure relaxation of crystal materials and compare different types of neural network architectures and reinforcement learning algorithms for this purpose. Experiments are conducted on Al-Fe structures, with potential energy surfaces generated using EAM potentials. We examine the influence of hyperparameter settings on model performance and benchmark the best-performing models against classical optimization algorithms. Additionally, the model's capacity to generalize learned interaction patterns from smaller atomic systems to more complex systems is assessed. The results demonstrate the potential of DRL models to enhance the efficiency of structure relaxation compared to traditional methods.