Working Group on Physics, Modern IT and Artificial Intelligence Arbeitskreis Physik, moderne Informationstechnologie und Künstliche Intelligenz (AKPIK)

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Overview of Sessions

(Lecture hall Theo 0.134; Poster ZHG Foyer 1. OG)

Sessions

AKPIK 1.1–1.3	Wed	13:45–14:45	ZHG001	**Theory of Machine Learning (joint session MP/AKPIK)**
AKPIK 2.1–2.2	Wed	16:15–18:15	ZHG Foyer 1. OG	**AKPIK Poster Session**
AKPIK 3.1–3.5	Thu	16:15–17:30	Theo 0.134	**Machine Learning in Particle- and Astroparticle Physics**
AKPIK 4.1–4.6	Fri	9:00–10:30	Theo 0.134	**Simulation and Workflows**

AKPIK 1: Theory of Machine Learning (joint session MP/AKPIK)

Time: Wednesday 13:45–14:45 Location: ZHG001

AKPIK 1.1 Wed 13:45 ZHG001

Time Series Analysis of machine learned Quantum Systems — •Kai-Hendrik Henk and Wolfgang Paul — Martin-Luther-Universität Halle-Wittenberg, Halle(Saale), Deutschland

The Rayleigh-Ritz variation principle is a proven way to find ground states and energies for bound quantum systems in the Schrödinger picture. Advances in machine learning and neural networks make it possible to extend it from an analytical search from a subspace of the complete Hilbert space to the a numerical search in the almost complete Hilbert space. Here, we extend the Rayleigh-Ritz principle to Nelson's stochastic mechanics formulation of non-relativistic quantum mechanics, and propose an algorithm to find the osmotic velocities $u(x)$, which contain the information of a quantum systems in this picture (*Phys. Rev. A 108, 062412*). Motivated by experiments by the Aspelmeyer group at the University of Vienna using quantum levitodynamics (see for example *Nature 595, 373-377 (2021)*), we apply the algorithm to the harmonic oscillator, the Gaussian and the Lorentzian potential and analyze them using methods from time series analysis and phase portraits.

References: *Henk, K.-H., and Paul, W. Machine learning quantum mechanical ground states based on stochastic mechanics. Phys. Rev. A 108 (Dec 2023), 062412*

AKPIK 1.2 Wed 14:05 ZHG001

Opening the Black Box: predicting the trainability of deep neural networks with reconstruction entropy — •Yanick Thurn[1], Ro Jefferson[2], and Johanna Erdmenger[1] — [1]Institute for Theoretical Physics and Astrophysics, Julius-Maximilians-University Wuerzburg — [2]Institute for Theoretical Physics, and Department of Information and Computing Sciences, Utrecht University

An important challenge in machine learning is to predict the initial conditions under which a given neural network will be trainable. We present a method for predicting the trainable regime in parameter space for deep feedforward neural networks (DNNs) based on reconstructing the input from subsequent activation layers via a cascade of single-layer auxiliary networks. We show that a single epoch of training of the shallow cascade networks is sufficient to predict the trainability of the deep feedforward network on a range of datasets (MNIST, CIFAR10, FashionMNIST, and white noise). Moreover, our approach illustrates the networks decision making process by displaying the changes performed on the input data at each layer, which we demonstrate for both a DNN trained on MNIST and the vgg16 CNN trained on the ImageNet dataset.

AKPIK 1.3 Wed 14:25 ZHG001

Analytic continuation of Greens functions with a neural network — •Martin Rackl, Yanick Thurn, Fakher Assaad, Anika Götz, René Meyer, and Johanna Erdmenger — Julius-Maximilians University Würzburg, Am Hubland, 97074 Würzburg, Germany

An important problem in many-body physics is to reconstruct the spectral density from the imaginary-time domain Greens function. Typically, this Greens function is generated by Monte Carlo methods. As the one-point fermionic kernel diverges for large frequencies, the numerical noise present generically causes instabilities. A standard method to tackle the reconstruction of the spectral density is the maximum entropy method (MaxEnt). In this paper, we follow a different approach and use a convolutional neural network for obtaining the spectral density for a given imaginary time Greens function. The network is very sensitive to the nature of the training data that we create using random Gaussians. Here we improve the training data set available by considering collision centres for Gaussians rather than uniformly distributed Gaussians. Our network is constructed in such a way that its output fulfils the positive semidefiniteness of the spectral density and is ppropriately normalized. We compare the results of this network with results of MaxEnt for the same problem. This comparison is performed for different cases: artificial test data, spin-charge separation in the 1d Hubbard model. Using the Wasserstein distance as metric, we find that the network performs in the same order of magnitude of accuracy as MaxEnt.

AKPIK 2: AKPIK Poster Session

Time: Wednesday 16:15–18:15 Location: ZHG Foyer 1. OG

AKPIK 2.1 Wed 16:15 ZHG Foyer 1. OG

Exploring GNN-based trigger algorithms for underwater neutrino telescopes — •Avalon Rego[1,2], Francesca Capel[2], Christian Spannfellner[3], and Li Ruohan[3] — [1]Ludwig-Maximilians-Universität, München, Deutchland — [2]Max-Planck-Institut für Physik, Garching bei München, Deutchland — [3]Technical University of Munich , Munich, Germany

Neutrinos are a window into a deeper understanding of both beyond standard model physics and various high-energy astrophysical phenomena. This is because they can easily escape dense environments due to their weakly interacting nature and can pinpoint their sources since they are not deflected by magnetic fields. We detect these weakly interacting particles by embedding detectors into massive volumes of naturally available water or ice and then detecting the Cherenkov radiation produced by their interactions. These detectors are sensitive to complex backgrounds such as bioluminescence signals which are a challenge for standard trigger algorithms. In this work we investigate the use of Graphnet, a GNN-based python framework, for signal classification and improving discrimination for bioluminescence signals in particular comparing it to a standard coincidence trigger. We also explore the possibility of using this trigger to lower the energy threshold for neutrino detection.

AKPIK 2.2 Wed 16:15 ZHG Foyer 1. OG

Automated Metadata Verification and Experimental Validation Using Dual Neural Networks in Alignment with FAIR Principles — •Rebekka Murati[1], Johannes Marczinkowski[1], Cedric Kessler[1], Andrei Schliwa[2], Matthias Böhm[3], and Nina Owschimikow[1] — [1]IOAP, TU Berlin — [2]IFKP, TU Berlin — [3]Institut für Softwaretechnik und Theoretische Informatik, TU Berlin

The sustainable management of scientific data is guided by the principles of Findability, Accessibility, Interoperability, and Reusability (FAIR). In particular, the quality and accuracy of metadata, data that describes the measurement data, play a central role in ensuring the reproducibility and integrity of experimental results. We present an approach for the automated verification and validation of metadata and experimental results, using the example of an X-ray spectroscopy experiment. The approach is based on the use of an electronic lab notebook and two neural networks for detecting data quality issues of both meta data and experimental data. We synthetically generated metadata (aligned with the FAIR principles) and a wide variety of measurement data, as well as introduced a spectrum of realistic data corruptions (e.g. spelling errors) for training these models. By combining both outputs, it becomes possible to make precise judgments about whether the metadata for the experiment has been fully and correctly recorded and whether the experiment itself was conducted without errors and is consistent with the metadata. This approach enables improved quality assurance and provides real-time feedback to experimenters regarding the quality of their data and metadata.

AKPIK 3: Machine Learning in Particle- and Astroparticle Physics

Time: Thursday 16:15–17:30 Location: Theo 0.134

AKPIK 3.1 Thu 16:15 Theo 0.134

A Hybrid Approach for Optimizing Background Simulations in IceCube — •Simon Koch, Christian Haack, and Benedikt Mayer — Erlangen Centre for Astroparticle Physics - ECAP, FAU Erlangen-Nürnberg

The IceCube Neutrino Observatory detects high-energy cosmic neutrinos by observing Cherenkov radiation emitted from secondary particles, such as muons, produced in neutrino interactions. A key challenge in detecting cosmic neutrinos is the large background of cosmic-ray induced muons, which has to be reduced by a factor of $\sim 10^7$.

Thus a large sample of background events has to be simulated in order to accurately estimate the background reduction efficiency. The computationally most expensive part of the simulation chain is the propagation of Cherenkov photons, induced by the muon energy losses.

In this work we develop a hybrid simulation approach that combines traditional simulation methods with a surrogate model. Our surrogate model predicts the probability of cosmic ray induced muons surviving the background reduction process based on the muon energy loss information. This approach ensures that computational resources required for the photon propagation of the background events are better spent on statistically rare events, which have a high chance of surviving the background reduction. For a given sample size of background events, we are thus able to reduce the statistical uncertainty of the estimated background reduction efficiency.

AKPIK 3.2 Thu 16:30 Theo 0.134

Searching for Ultra-High Energy Photons applying Machine Learning Methods Using the Surface Detector of the Pierre Auger Observatory — •Fiona Ellwanger for the Pierre-Auger-Collaboration — KIT, Karlsruhe, Germany

Identifying sources of cosmic rays is challenging, as the charged particles are deflected by magnetic fields and do not point back to their sources. Neutral particles, such as ultra-high energy (UHE) γ's will point directly to their sources, unless they interact in the interstellar medium or are absorbed. Cosmic ray detectors such as the 3000 km^2 surface array of the Pierre Auger Observatory are capable of observing UHE γ's above 10^{18} eV. With increasing energy, their mean free path allows probing extragalactic sources up to a few Mpc. Unlike cosmic rays, photon-induced showers are almost purely electromagnetic. Different methods like BDTs and air-shower Universality have been previously applied to the search of γ's at different energy ranges. Although no UHE γ's have been found, the obtained bounds of the fluxes provide crucial constraints on cosmic-ray acceleration models.

Neural networks have the potential to improve discriminating variables, enhancing the sensitivity to even lower fluxes. In this work, we present a convolutional neural network designed to distinguish between simulated UHE photon and proton showers. We evaluate it on an independent test set, assessing its sensitivity and robustness to systematic uncertainties, including broken stations, detector aging, and noise. These steps aim to validate the network for application to the measured events.

AKPIK 3.3 Thu 16:45 Theo 0.134

Neural Network-Based Event-by-Event Reconstruction of Muon Number from Data of the SD-750 of the Pierre Auger Observatory — •Alina Klingel for the Pierre-Auger-Collaboration — KIT, Karlsruhe, Deutschland

Ultra-high-energy cosmic rays ($\sim$ 1 EeV) provide a unique opportunity to probe physics beyond the energies of human-made accelerators. At such extreme energies, direct detection is infeasible; instead, these cosmic rays are studied through the particle cascades, or air showers, they generate upon interacting with Earth's atmosphere. The SD-750 surface detector of the Pierre Auger Observatory records the shower footprint, the spatial distribution of particles and energy deposited on the ground, as time-resolved ground signals. The main advantage of the SD-750 lies in its proximity to the Underground Muon Detector (UMD), allowing for an independent measurement of the muon content of air showers. This setup forms an ideal testbed to develop and benchmark neural network-based estimators for the muon number, even when simulations contain discrepancies. In this contribution, we present a neural network architecture designed to predict the relative muon number in air showers. We aim to shed light on the muon puzzle by cross-calibrating with muon measurements from the UMD.

AKPIK 3.4 Thu 17:00 Theo 0.134

Advanced Northern Tracks Selection using a Graph Convolutional Neural Network for the IceCube Neutrino Observatory: Adversarial Training — •Leon Hamacher, Philipp Behrens, Jakob Böttcher, Shuyang Deng, Lasse Düser, Philipp Fürst, Philipp Soldin, and Christopher Wiebusch for the IceCube-Collaboration — RWTH Aachen

The IceCube Neutrino Observatory, located at the South Pole, detects atmospheric and astrophysical neutrinos. One important task is differentiating between these neutrinos and muons induced by air showers. The Advanced Northern Tracks Selection (ANTS) accomplishes this identification using a graph-convolutional neural network. However, neural networks can be sensitive to minor adversarial perturbations, which can significantly alter their outputs. Adversarial training is a method to include artificially perturbed data during the training process to enhance resistance to such perturbations. For this purpose, a dedicated algorithm, MiniFool, has been developed that takes experimental uncertainties into account. This talk presents the results of applying MiniFool to ANTS.

AKPIK 3.5 Thu 17:15 Theo 0.134

Adaptive Generative Modeling for Accelerated Calorimeter Simulations via Domain Transfer — •Lorenzo Valente[1], Fank Gaede[2], Gregor Kasieczka[1,3], and Anatolii Korol[2] — [1]Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Deutsches ElektronenSynchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany — [3]Center for Data and Computing in Natural Sciences CDCS, Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, 22607 Hamburg, Germany

Simulating particle collider detectors presents significant computational challenges, with current methods struggling to scale with increasingly complex experimental datasets. Deep generative models offer a promising solution for dramatically reducing computational overhead, especially as upcoming particle physics experiments are expected to produce unprecedented volumes of data.

We introduce a novel domain adaptation framework that utilises state-of-the-art deep generative models to generate high-fidelity 3D point-cloud representations of particle showers. Using transfer learning techniques, our approach adapts simulations across diverse electromagnetic calorimeter geometries with exceptional data efficiency, thereby reducing training requirements and eliminating the need for a fixed-grid structure.

Preliminary results demonstrate that our method can achieve high accuracy while significantly reducing data and computational demands, offering a scalable solution for next-generation particle physics simulations.

AKPIK 4: Simulation and Workflows

Time: Friday 9:00–10:30 Location: Theo 0.134

AKPIK 4.1 Fri 9:00 Theo 0.134

Integration of a data centre for high-energy astroparticle physics in PUNCH4NFDI infrastructure — •Victoria Tokareva — Karlsruhe Institute of Technology, Institute for Astroparticle Physics, 76021 Karlsruhe, Germany

The PUNCH4NFDI (Particle, Universe, NuClei and Hadrons for Nationale Forschungsdaten Infrastruktur) consortium brings together experts from astro-, nuclear, astroparticle and particle physics to develop an infrastructure and tools for data-intensive research. The PUNCH4NFDI Science Data Platform (SDP) aims to provide users with access to the data resources of the data providers participating in the consortium, while offering advanced features such as enhanced search capabilities for data objects, support for reproducible workflows, and online data analysis.

One such data provider is the KCDC (KASCADE Cosmic-ray Data Centre). Established in 2013, KCDC was the first online platform to provide full open access to data from the high-energy astroparticle physics experiment KASCADE and its successor KASCADE-Grande. Over time, its scope expanded to include data from other astroparticle physics experiments as well as a wider range of digital objects such as simulations, software codes, user manuals, tutorials, and cosmic-ray spectra. This contribution shows the status of the integration of KCDC's data objects into the PUNCH4NFDI SDP, addresses encountered challenges, and describes strategies and technical solutions chosen for this purpose. This work is partially supported by the DFG fund 'NFDI 39/1' for the PUNCH4NFDI consortium.

AKPIK 4.2 Fri 9:15 Theo 0.134

The Lecture Notes Makeover with AI — •Soraya Thiess, Ilya Segal, and Mikhail Mikhasenko — Ruhr University Bochum, Bochum, Germany

Artificial intelligence is rapidly advancing, offering powerful tools to automate and enhance various workflows. This research project aims to accelerate the creation of scientific scriptures with the use of Large Language Models (LLM). We use a programming interface (API) to an advanced LLM provided by OpenAI to transform raw lecture material, like audio transcriptions and handwritten notes, into well-phrased and organized formats. In a multi-step process, beginning with the segmentation of the input into distinct topics, the content gets rephrased to enhance readability while ensuring contextual accuracy by addressing any out-of-place terminology. The user can choose the desired output format, such as Markdown or LaTeX, and incorporate images afterwards. While designed for the input of audio transcriptions and notes of hadronphysics lectures, this model could be adapted for any field requiring the transformation of spoken or handwritten content into structured, publication-ready material.

AKPIK 4.3 Fri 9:30 Theo 0.134

Parametrizing workflows with ParaO and Luigi — Martin Erdmann and •Benjamin Fischer — III. Physikalisches Institut A, RWTH Aachen University

Workflow tools provide the means to codify complex multi-step processes, thus enabling reproducibility, preservation, and reinterpretation efforts. Their powerful bookkeeping also directly supports the research process, especially where intermediate results are produced, inspected, and iterated upon frequently.

In Luigi, such a complex workflow graph is composed of individual tasks that depend on one another, where every part can be customized at runtime through parametrization. However, Luigi falls short with regards to the steering of parameters, accounting for the consequences thereof, and the modification or reuse of task graphs.

This is where the parameter handling of ParaO shines: it has vastly extended key mechanics and value coercion while automatically propagating their effects throughout the task graph. Since the dependencies are described through parameters too, the same principles can be used to freely alter or transplant (parts of) the task graph, thereby empowering reuse. At the same time, ParaO remains largely compatible with plain Luigi and packages building upon it, such as Law.

AKPIK 4.4 Fri 9:45 Theo 0.134

Simulation of radio galaxies with 2D Gaussian distributions — •Christian Arauner, Anno Knierim, Tom Gross, and Kevin Schmitz — TU Dortmund University, Dortmund, Germany

Radio interferometry enables high-resolution observations of astronomical objects. Due to the incomplete coverage of the (u, v) space, these observations are very noisy. The state of the art cleaning algorithms are time-consuming and not scalable for the expected data volumes of the next gen telescopes As an alternative, neural networks can be used, which can automate and accelerate the cleaning of many measurements. However, training a neural network requires large amounts of training data that have the same properties as the observed objects.

Due to the fact that neural networks are a new approach, there are still very few simulations of training data. The observations from the MOJAVE archive are particularly suitable for the development of simulation software. The archive comprises a large data set of high-quality data that has been measured over a long period of time under similar conditions. The individual components of the galaxies can be generated with multidimensional Gaussian distributions, and a complete galaxy can be simulated from the sum of the components.

In this talk, I will present a novel approach to simulate radio galaxies with multidimensional Gaussian distributions.

AKPIK 4.5 Fri 10:00 Theo 0.134

Simulating Polarisation in Radio Interferometry Experiments Using pyvisgen — •Anno Knierim, Christian Arauner, and Kevin Schmitz — TU Dortmund University, Dortmund, Germany

Recent approaches in radio astronomy aim to improve image cleaning in radio interferometry measurements using machine learning techniques. Reconstructing sources using these novel techniques has the advantage of being agnostic to initial parameters used in traditional cleaning algorithms.

The radionets project is a deep-learning framework developed at TU Dortmund University. The goal is to reconstruct calibrated observations with convolutional neural networks to produce high-resolution images. Deep learning approaches such as radionets require large amounts of training and validation data. One approach to simulating the required datasets is provided by the simulation tool pyvisgen.

pyvisgen utilises the Radio Interferometer Measurement Equation (RIME) to represent the measurement process of a radio interferometer. It produces images suitable as input to train deep-learning-based cleaning approaches. This talk presents the recent implementation of polarisation effects on radio waves.

AKPIK 4.6 Fri 10:15 Theo 0.134

Binary Black Hole Parameter Estimation using a Conditioned Normalizing Flow — •Markus Bachlechner and Achim Stahl — III. Physikalisches Institut B, RWTH Aachen

The proposed Einstein Telescope is the first of the third-generation gravitational wave detectors. It is expected to reach a noise level at least an order of magnitude lower than current interferometers like LIGO and Virgo. The thus improved sensitivity increases the observable volume and extends the time window in which the inspiral phase of binary systems is measurable. To analyze the resulting vast amounts of data efficiently, Neural Networks (NNs) can be utilized. This talk presents a fast Binary Black Hole parameter reconstruction by applying a conventional convolutional NN which conditions a subsequent Normalizing Flow (NF). Using the NF, an approximated posterior parameter distribution on an event-by-event basis is obtained, and thus uncertainties can be estimated.