Book of abstracts
Postersessions of the ASC school 2022
"Physics meets AI"

Tuesday, September 13

1. **Symmetry-protected Bose-Einstein condensation of interacting hardcore bosons**

   Reja Helene Wilke

   We introduce a mechanism stabilizing a one-dimensional quantum many-body phase, characterized by a certain wave vector via the protection of an emergent Z2 symmetry. We illustrate this mechanism by constructing the solution of the full quantum many-body problem of hardcore bosons on a wheel geometry, which are known to form a Bose-Einstein condensate. The robustness of the condensate is shown numerically by adding nearest-neighbor interactions to the wheel Hamiltonian. We discuss further applications such as geometrically inducing finite-momentum condensates.

2. **Limits and prospects of molecular fingerprinting revealed through in silico and predictive modeling**

   Tarek Eissa

   Molecular fingerprinting by vibrational spectroscopy can effectively characterize the chemical composition of complex organic media. By exciting the molecular constituents contained within, infrared spectrometers produce spectra which reflect light-matter interactions. Pattern recognition algorithm are capable of discerning between measurements of different sample states and enable spectral phenotyping – the identification of spectral biomarkers to classify "diseased" samples. Although such applications have been successfully showcased, the fundamental possibilities and limitations of the approach remain largely unexplored. To address this, we developed an in silico model which generates realistic, but configurable, spectra that factor in the effects of multiple sources of noise influencing spectral measurements. By systematically varying the parameters of our simulation model, we apply machine learning methods to detect lung cancer from blood-based samples and investigate how variations in experimental designs, focusing on sources of measurement noise, affect classification performance. Our study contributes towards establishing a framework to strengthen our understanding of spectral phenotyping and exposes opportunities for future molecular fingerprinting applications.

3. **Inferring the assembly and merger histories of galaxies with the IllustrisTNG simulations and machine learning**

   Lukas Eisert

   What information can one infer about a galaxy from observations? We uncover the connections between observable and unobservable properties of galaxies, with a focus on their unobservable past merger and assembly history. To do so, we use full cosmological simulations to track galaxies as they evolve with time. We use machine learning algorithms to transfer the information from the simulated galaxies to observed ones. We develop two complementary approaches; either using observable scalar quantities or Hyper-Suprime-Cam Images.

4. **Uncertainty Quantification for Multiscale Turbulent Transport Simulations of a Magnetic Confinement Fusion Device using Machine Learning Surrogate Models**

   Yehor Yudin

   One of the challenges in understanding the energy and particle transport processes in the core plasma of a magnetic confinement fusion device is to quantify how it is effected by turbulent dynamics. This work considers a multiscale approach of modelling this problem, where models of processes on different spatial and temporal scales are coupled to obtain the numerical solution. Furthermore, the resulting model is used to investigate both epistemic and aleatoric uncertainties in the profiles of the transported quantities. This work proposes application of a surrogate modelling technique to reduce the computational cost of resolving a quasi-steady state solution on the microscale when it is sufficient to capture only statistics of turbulent dynamics. We studied a Multiscale Fusion Workflow that utilizes turbulent energy and particle fluxes computed with a gyrofluid turbulence code GEM in flux tube approximation to calculate the transport coefficients for a core transport code ETS. In this work, a data-driven probabilistic surrogate model based on Gaussian Process Regression is used to infer flux values computed by a turbulence code for given core profiles, and to calculate related uncertainties. For that, we use VECMA toolkit to perform uncertainty quantification, as well as to train, test and utilize surrogate models.

5. **Optimizing the classification of biological tissues using polarized data supported by Machine Learning**

   Carla Rodríguez

   Polarimetric data is nowadays used to build recognition models for the characterization of organic tissues or the early detection of some diseases. We present a thorough comparative between classification models based on different polarimetric data basis, this allowing us to find the ideal polarimetric framework to construct tissue classification models. Four different well-known classificatory algorithms are compared by analyzing three polarimetric datasets: (A) a selection of most representative polarimetric observables presented in literature; (B) Mueller matrix coefficients; and (C) the combination of (A) and (B) sets. The study is conducted on the experimental Mueller matrices images measured on different organic tissues: muscle, tendon, myotendinous junction and bone; all of them measured from a collection of 165 ex-vivo chicken thighs. The presented methods may be of interest in multiple biological applications.

6. **Relative entropy in neural networks**

   Yanick Thurn

   Using methods from quantum field theory and quantum information theory we try to improve the training of neural networks. We introduce a new way to use the Kullback-Leibler divergence to get insight into the training of neural networks. The Kullback-Leibler divergence, also known as relative entropy, can be seen as a distance measure between probability distributions. Similar to restricted Boltzmann machines, the relative entropy is calculated between two different activations in the same layer instead of neighboring layers, whereas the second activation is determined by a new propagation method we introduce. Intuitively, it can be seen as propagating the most important features to the next layer and, subsequently, back to the original one. This allows a comparison of the transported information between layers. We refer to this approach as reflective relative entropy (RRE). In the large-N limit, the trainability of neural networks depends on different parameters including the variance of the weights and biases while initialization. This results in a phase diagram, where the trainability of the network seems to be optimal close to the critical point. A relation between the RRE and the critical phase is observed. This indicates a phase sensitivity of the RRE, which could be used to improve the training of neural networks.

7. **Reservoir Computing with Many-Body Simulations**

   Mario Gaimann

   Spatio-temporal prediction of chaotic systems is a challenging problem that is relevant for many fields (weather, finance, energy, and other dynamic systems) [1]. Recurrent neural networks and specifically reservoir computers were previously used to approach this problem [2]. However, these learning systems are typically treated as black boxes, and do not incorporate physical reasoning in terms of physical laws and dynamics. Here we present a novel approach where we use simulations of physical systems as reservoirs. This allows us to determine and interpret the state of our reservoir in physical terms and relate the learning problem to other generic phenomena in statistical physics. With this knowledge we aim to understand optimal conditions for learning in relation to critical states, external driving, and physical constraints. We shall try our reservoir using a broad range of physical systems – simple swarm intelligence models [3] or hard rod models [4], for instance. Our simulations may inspire hardware implementations and the development of new devices for unconventional computing. References: [1] Schrauwen, B. et al. (2007). ESANN 2007 Proceedings, 471–482. [2] Lukoševičius, M. et al. (2012). KI - Künstliche Intelligenz 26(4), 365–371. [3] Lymburn, T. et al. (2021). Chaos 31(3), 033121. [4] Quiring, P., Klopotek, M., Oettel, M. (2019). Physical Review E 100(1), 012707.

8. **Design of a deep neural network suitable for real-time feedback strategies discovered via reinforcement learning on a quantum device**

   Jonas Landgraf

   Real-time feedback for quantum systems is an essential ingredient in many quantum control tasks, such as quantum error correction and quantum state preparation. Two aspects make feedback challenging: First, a time far shorter than the coherence time is required. Second, it represents a complex decision making problem. The subfield of machine learning dealing with optimizing strategies for problems of this type is reinforcement learning, whose power has been convincingly demonstrated in areas ranging from robotics to video and board games. In this work, we present and analyze the design of a neural network which can be implemented on a Field Programmable Gate Array (FPGA) to discover real-time feedback strategies for initialization of a superconducting qubit. Our network will be trained via reinforcement learning which is only based on data directly accessible in an experiment, such that precise knowledge of the underlying dynamics is not required. To address the challenge of low latency, we introduce a key idea: the network inference computation is interleaved with the simultaneous collection of measurement data.

9. **Can Artificial Intelligence Improve the Simulation of Realtime Dynamics of Quantum Fields in NISQ Era?**

   Chinonso Onah

   One of the most promising areas for quantum computing is in simulation of the dynamics of interacting quantum systems. This is also an area where Quantum Advantage in NISQ era is likely to be realized. In the absence of Error Correction, we investigate whether Machine Learning based error mitigation strategies can improve the simulation of the dynamics of Quantum Fields on NISQ devices. Using error mitigation strategies, HuffMan, Vera, and Banerjeewe benchmarked real time dynamics of Z2 and U(1) gauge invariant plaquette models using superconducting-qubit based quantum IBM Q computers. Here, we investigate how this could be improved with Machine Learning based error mitigation strategies and further apply error mitigation to other species of quantum fields.

10. **Antifragile Persistent Homology using Fisher Information**

    Karthik Viswanathan

    Persistent Homology (PH) computes the topology of datasets at different length scales. It is observed that PH contains an informative summary of the observables in various physical systems. I will present how this technique can be made adaptive by learning the optimal filtration that is resilient to noise in data. This is done by maximizing the Fisher Information among a variational family of filtration parameters using gradient descent. By doing so, we construct an informative persistence diagram and consequently, a compressed summary of the input data that is sensitive to the input parameters.

11. **Physics solutions for machine learning privacy leaks**

    José Ramón Pareja Monturiol

    Machine learning systems are becoming more and more ubiquitous in increasingly complex areas, including cutting-edge scientific research. The opposite is also true: the interest in better understanding the inner workings of machine learning systems motivates their analysis under the lens of different scientific disciplines. Physics is particularly successful in this, due to its ability to describe complex dynamical systems. While explanations of phenomena in machine learning based on physics are increasingly present, examples of direct application of notions akin to physics in order to improve machine learning systems are more scarce. Here we provide one such application in the problem of developing algorithms that preserve the privacy of the manipulated data, which is especially important in tasks such as the processing of medical records. We develop well-defined conditions to guarantee robustness to specific types of privacy leaks, and rigorously prove that such conditions are satisfied by tensor-network architectures. These are inspired by the efficient representation of quantum many-body systems, and have shown to compete and even surpass traditional machine learning architectures in certain cases. Given the growing expertise in training tensor network architectures, these results imply that one may not have to be forced to make a choice between accuracy in prediction and ensuring the privacy of the information processed.

12. **Bidirectional optimal quantum control boosted by deep learning: A use case of polarization in liquid crystals**

    Dominik Vašinka

    Quantum devices share the common aspect of being controlled by classical analog signals, related nontrivially to the device operation. The control signals need to be optimally adjusted to provide a high-fidelity operation of the device. A common approach to predicting control signals required to prepare the target quantum state, i.e., the inverse control model, minimizes an ad hoc selected distance metric in the classical control space. However, the values of control signals are given by the technical implementation and are often ambiguous. We propose and experimentally test a novel idea for constructing the inverse control model. We develop an unsupervised-like deep learning approach combining the inverse and direct control models. The classical control signals play the role of latent variables with no required quantification in the latent space. By minimizing the error in the space of quantum states, various models and devices, even with a different number of control signals, can be optimized and compared. We demonstrate our approach on a use case of polarization state transformation using twisted nematic liquid crystals controlled by several voltage signals. Furthermore, the method is used for the preparation and remote preparation of polarization-encoded qubits with unprecedented accuracy.

13. **Classifying Anomalies THrough Outer Density Estimation (CATHODE)**

    Manuel Sommerhalder

    We propose Classifying Anomalies THrough Outer Density Estimation (CATHODE): A novel, fully data-driven and model-agnostic approach to detect resonant new physics with anomalous jet substructure at the LHC. Training a conditional normalizing flow on substructure variables in a sideband region, we obtain an approximation of their probability densities. We then interpolate our trained background model into the signal region and sample from it, which yields an estimation of the standard model background inside the signal region without relying on a full simulation. Finally, a neural network classifier is trained to distinguish data events from the sampled background within the signal region in order to detect overdensities caused by an anomalous new physics signal. Using the LHC Olympics R&D dataset as benchmark, we report an improvement of the nominal statistical significance from $\sim 1\sigma$ to as much as $\sim 15\sigma$. Thus, the CATHODE method is able to discover new physics that otherwise would be hidden in data.

14. **How Machine Learning Helps to Find Efficient Organic Photocatalysts for Hydrogen Generation**

    Viola Steidl

    Organic semiconductors are promising candidates for photocatalytic hydrogen evolution. In particular, π-conjugated polymers have many advantages over inorganic semiconductors: they are environmentally friendly, contain earth-abundant elements, can be synthesized under mild conditions, and their properties are easily tunable.[1] However, the compositional variety of polymers makes it challenging to evaluate their performance experimentally. In collaboration with the ARC Centre of Excellence in Exciton Science in Melbourne, Australia, we developed an unsupervised and supervised machine learning method to classify polymers according to their H2 evolution rate. An autoencoder network generates a set of abstract descriptors based on a database of polymers.[2] These features are then used to train a classifying neural network on a subset of polymers with known hydrogen evolution rates. The classification of polymers into high and low performers reduces the number of experiments needed to find highly active materials. Importantly, photocatalytic measurements demonstrate that the model successfully predicts a highly efficient polymer from the overall dataset. References: [1] J.K. Stolarczyk et al, ACS Catalysis. Vol. 8, 3602-3635 (2018). [2] Y. Bai et al, Journal of the American Chemical Society. Vol. 141, 9063-9071 (2019). [3] V. Steidl et al, in preparation

15. **Stable fusion turbulence simulations through hybrid numerical-AI methods**

    Robin Greif

    Recent progress in hybrid numerical and data driven methods have shown great promise for computational fluid dynamics (CFD). In this work we extend their applicability to simulating turbulence in nuclear fusion reactors, endlessly stable physical simulations of drift wave turbulence are possible with discretizations previously unfeasible. With empirical speedups over 3 orders of magnitude, this approach bears big promise for reducing the complexity and resource hunger of the push for practically endless clean energy through nuclear fusion.

16. **Validation of quasilinear transport models in the ASTRA framework**

    Michael Bergmann

    By combining multiple heating and transport subroutines ASTRA is capable of simulating realistic temperature and density radial profiles of fusion plasmas. While these profiles match experimental data taken from e.g. the Integrated Data Analysis (IDA) code, the simulated gradients often differ from measured ones and are largely dependent on the turbulence subroutine chosen. The interest in correct plasma gradients is particularly high as these give rise to the turbulence which dominates the transport. Using two quasi-linear turbulence solvers (TGLF and Qualikiz) as well as their much faster neural-network versions we shall explore the validity and uncertainty of the models in different discharge scenarios via input-error propagation, as well as comparing the models to high-fidelity codes such as GENE and experimental measurements. This work feeds back into attempts of using ASTRA simulations as a theoretical prior for IDA, where the prior of the simulated profile is needed.

17. **Identification of mature thunderstorms in NWP simulations using artificial neural networks**

    Kianusch Vahid Yousefnia

    Thunderstorms constitute a major hazard to society and economy. Especially in light of the expected increase of extreme weather events due to climate change, thunderstorm forecasts become ever more important. One way of solving the forecast problem within the accuracy of the numerical solver consists of identifying thunderstorms in forecast data. To this end, we present a method of identifying signatures of mature thunderstorms in numerical weather prediction (NWP) simulations using a feedforward artificial neural network (ANN). The aim is to infer the probability of thunderstorm occurrence at some point in space and time, given only a set of local input parameters that are extracted from NWP simulations and related to thunderstorm development. We start by introducing crucial conceptual principles of the thunderstorm identification problem, some of which have not been sufficiently discussed in the literature. This includes in particular the choice of input parameters, the labelling of thunderstorm regions and a mathematically sound definition of a likelihood score of thunderstorm occurrence. In order to train the neural network, ensemble forecasts of ICON-D2-EPS with lead times of at most two hours are used to procure hourly values of the input parameters for Central Europe from May to October 2021. Lightning data collected through the LINET network serve as labels for classifying whether a mature thunderstorm occurs for a given set of input parameters in the training dataset. We measure the identification skill of our neural network by determining the percentage of correctly identified thunderstorm events and false alarms in a test dataset. Even with a relatively simple ANN-architecture and local input parameters, we find an identification skill superior to comparable approaches in the literature.

18. **Symmetries, Safety, and Self-Supervision**

    Lorenz Vogel

    Collider searches face the challenge of defining a representation of high-dimensional data such that (i) physical symmetries are manifest, (ii) the discriminating features are retained, and (iii) the choice of representation is data-driven and new-physics agnostic. We introduce JetCLR (Contrastive Learning of Jet Representations) to solve the mapping from low-level jet constituent data to optimized observables through self-supervised contrastive learning. Using a permutation-invariant transformer-encoder network, physical symmetries such as rotations and translations are encoded as augmentations in a contrastive learning framework. As an example, we construct a data representation for top and QCD jets and visualize its symmetry properties. We benchmark the JetCLR representation against other widely-used jet representations, such as jet images and energy flow polynomials (EFPs).

19. **MLOps for High Energy Physics**

    Daniel Holmberg

    Usage of machine learning has seen a dramatic increase in many domains including high energy physics. It is however a challenging task to bring ML products into production, not to mention in an automated fashion. Furthermore, ML is often reliant on the availability of hardware accelerators such as GPUs which are in scarce availability to accelerate model training. To address these points the IT department at CERN has deployed a platform called Kubeflow aimed at managing the full machine learning lifecycle while being resource efficient. An example particle physics usecase from the CMS experiment is run on the platform introducing the different components of the platform such as Katib AutoML and scalable serving over http.

20. **Operator Inference - a non-intrusive reduced-order modeling framework for plasma simulations**

    Constantin Gahr

    Simulations play a crucial role in the plasma physics community as they give insight into otherwise unobservable structures and dynamics. However, they are computationally expensive and take a long time to run. In contrast, reduced-order models sacrifice accuracy for simulation speed and reduced complexity by solving a reduced-order approximation instead of the full PDE. However, they are often intrusive or not able to model the non-linear laws guiding the plasma. Operator Inference is a model reduction method that is both non-intrusive and able to handle arbitrary non-linearities. As such, it is a potential candidate for model reduction in the context of plasma physics. Operator Inference learns a reduced-order approximation of the original differential equation by fitting a reduced model to the data. This reduced-order model approximates the Galerkin projection of the high order model onto its truncated singular value decomposition. In addition, Operator Inference can embed arbitrary non-linearities. Thus, it is the perfect candidate for modeling non-linear plasma dynamics and embedding the underlying physical laws guiding the plasma into the reduced space.

21. **IEA-GAN: Intra-Event Aware GAN with Relational Reasoning for the Fast Detector Simulation**

    Hosein Hashemi

    A realistic detector simulation is extremely important in particle physics. Currently it is very inefficient computationally as large amounts of resources are required for the production, storage and distribution of simulation data. Deep generative models allow for more effective fast simulation of this data. Nevertheless, generating detector responses is a highly non-trivial task as they carry fine-grained information and have correlated mutual properties within an “event”, a single readout window after the collision of particles. Thus, we propose the Intra-Event Aware GAN (IEA-GAN), in order to generate sensor-dependent images for the Pixel Vertex Detector (PXD) which is the sub-detector with the highest spacial resolution at the Belle II Experiment. First, we show that using the domain-specific relational inductive bias by introducing a Relational Reasoning Module, one can approximate the concept of an event in the detector simulation. Second, we incorporate a Uniformity loss in order to maximize the information entropy of the discriminator’s knowledge. Lastly, we develop an Intra-Event Aware loss for the generator in order to imitate the dyadic class-to-class knowledge of the discriminator. As a result we show that the IEA-GAN not only captures fine-grained semantic and statistical similarity among the images, but also finds correlation among the them. Ultimately, It also leads to a significant enhancement in the image fidelity and diversity in comparison to previous state of the art models.

22. **CO2 emissions from physics research?**

    Anna Knörr

    Climate change is relevant to everyone, we must all think together about how to reshape our communities towards net-zero operations. This interactive poster is part of an ongoing effort to address how climate change impacts the physics community, specifically, and serves a twofold aim: Firstly, spreading awareness for the orders of magnitude of the issue. Secondly, providing a space for people to voice their concerns, debate different solution approaches and add their own. Post-its are provided!

Thursday, September 15

1. **Representing neural activity using quantum generative adversarial networks**

   Vinicius Fonseca Hernandes

   Understanding how information is processed in biological neural networks is one the biggest challenges in modern science, with results that can greatly impact the fields of neuroscience, deep learning and information theory. It's understood reasonably well how an individual neuron works, and even if a single biological neuron is way more complex than its "silicon counterpart", several simplified computational models - such as the McCulloch-Pitts neuronal model, or the perceptron - have showed great potential when modelling how information is transferred between neurons, setting the fundamentals for the development of very complex pattern-recognition models with great predictive power. Another important step towards achieving a better comprehension of the brain is accurately modelling neuronal activity, which makes it possible to study properties such as network connectivity or response to stimuli, in a controlled environment. Efficient computational models for neuronal activity are hard to engineer, since the number of states they have to represent scales exponentially with the network size. Several approaches achieved efficient models that reproduce properties like network connectivity with very high precision [1,2]. However, they still demand a high number of parameters to simulate very large systems, making them complex to be analyzed. In this work we propose a novel approach to model neuronal activity using Quantum Generative Adversarial Network (QGAN) [3], the quantum equivalent to Generative Adversarial Networks [4], where a generative network is used to produce data that mimic the real data one wants to simulate, and a discriminative network is trained to distinguish between the synthetic data produced by the generative network, and the real one. The result of such architecture is that, after being trained, the generative network can produce samples indistinguishable from the real data. The advantage introduced by QGAN is to use a parameterized quantum circuit (PQC) [5] as the generative network, exploiting the fact that the number of degrees of freedom a quantum system encodes scales exponentially with the system size. Using this property we can efficiently encode all the possible states the neuronal network can assume - specifically, since each neuron can be active or inactive, the number of possible states for a neuronal network with N neurons is 2N. We encode each one of this possible states in the amplitudes of the PQC used as the generative network. Then, the generative circuit will be trained together with a (classical) discriminative network, in an adversarial manner, until it starts producing synthetic data that match the same statistics as those observed in the real one, when can then be used to simulate new samples, and since the model is very compact, its correlations can be easily analyzed, leveraging our knowledge about how information is processed in neuronal networks. The experimental data considered for neuronal activity consists of spike trains extracted from microelectrode arrays (MEA) measurements [6], taken from cultures of hippocampal cells from mouse embryos. We developed a Python framework that post-process the raw data obtained from measurements. The first and most important quantity extracted from neuronal activity signal is spike trains, which indicate when regions of the neuronal network are active, and when not. Spike trains can be used to detect bursts, another important quantity that can be used to calculate statistics about the network activity state. A common approach to detect bursts in MEA recordings is to use the MaxInterval Method [7], which uses spike trains and several tunable parameters to define when bursts are attributed to specific recording times. One problem with this method is that is hard to define the best set of tunable parameters that return reliable bursts, and constantly these parameters have to be manually tuned for individual datasets. In our framework, a convolutional neural network is used to predict optimal values for the MaxInterval parameters. This model can be used to treat real data, from MEA recordings, but also spike trains generated by the QGAN model, facilitating the comparison between the statistics observed in real and synthetic data. References: [1] A. Tang, D. Jackson, J. Hobbs, W. Chen, J. L. Smith, H. Patel, A. Prieto, D. Petrusca, M. I. Grivich, A. Sher, P. Hottowy, W. Dabrowski, A. M. Litke, and J. M. Beggs. A maximum entropy model applied to spatial and temporal correlations from cortical networks in vitro. Journal of Neuroscience, 28(2):505–518, 2008. [2] C. O'Donnell, J. T. Gonçalves, N. Whiteley, C. Portera-Cailliau, and T. J. Sejnowski. The Population Tracking Model: A Simple, Scalable Statistical Model for Neural Population Data. Neural Computation, 29(1):50–93, 2017. [3] P. Dallaire-Demers and N. Killoran. Quantum generative adversarial networks. Phys. Rev. A, 98:012324, 2018. [4] I. Goodfellow, J. Pouget-Abadie, M. Mirza, B. Xu, D. Warde-Farley, S. Ozair, A. Courville, and Y. Bengio. Generative adversarial nets. Advances in Neural

Information Processing Systems, 27. Curran Associates, Inc., 2014. [5] M. Benedetti, E. Lloyd, S. Sack, and M. Fiorentini. Parameterized quantum circuits as machine learning models. Quantum Science and Technology, 4(4):043001, 2019. [6] M. E. J. Obien, K. Deligkaris, T. Bullmann, D. J. Bakkum, and U. Frey. Revealing neuronal function through microelectrode array recordings. Frontiers in Neuroscience, 8, 2015. [7] C. R. Legendy and M. Salcman. Bursts and recurrences of bursts in the spike trains of spontaneously active striate cortex neurons. Journal of Neurophysiology, 53(4):926–939, 1985.

2. **SwarmRL: Active Colloids meet Reinforcement Learning**

   David Zimmer

   In this poster, we present SwarmRL, a Python package for the study of active matter using reinforcement learning and classical algorithms. SwarmRL is built to be run in both a simulation environment, powered by the ESPResSo engine, or in a real experimental setup. This poster demonstrates some of the capabilities of the SwarmRL engine including classical policies, reinforcement learning options, and the simplicity of use.

3. **Can linear regression predict parameters for measuring a disordered quantum device?**

   Sathish Kumar Rangaswamy Kuppuswamy

   A scalable spin-based quantum processor requires a suitable semiconductor heterostructure and a gate design, with multiple alternatives being investigated. Characterizing such devices experimentally is a demanding task, with the full development cycle taking at least months. While numerical simulations are more time-efficient, their predictive power is limited due to unavoidable disorder and device-to-device variation. We develop a spin-qubit device simulation for determining the coupling strengths between the electrostatic gate potentials and the effective device Hamiltonian in presence of disorder. By comparing our simulation results with the experimental data, we demonstrate that the gate couplings match up to disorder-induced variance. To demonstrate the flexibility of our approach, we also analyze an alternative non-planar geometry inspired by FinFET devices. Having achieved close agreement with the experiments at a reasonable time efficiency, we can predict gate designs for spin qubit devices robust to disorder based on simple machine learning algorithms such as linear regression.

4. **Anomaly Detection in Mass Spectrometry Data of Water Samples**

   Viktoria Maike Paula Pauw

   We analyze Non-Target Screening data of Samples of River and Lake water obtained with Liquid Chromatography - High Resolution Mass Spectrometry to find footprints of unusual chemical properties and pollutants. We present the approaches using machine learning techniques like Autoencoders and Decision Trees explored in the research project K2I from the Digital Green Tech Initiative (funded by BMBF) conducted at Leibniz-Rechenzentrum.

5. **Adaptive Quantum State Tomography with Active Learning**

   Hannah Lange

   Recently, tremendous progress has been made in the field of quantum science and technologies: platforms for quantum simulation as well as quantum computing, ranging from superconducting qubits to neutral atoms, are starting to reach unprecedentedly large systems. An efficient tool to gain insights into such large quantum systems is quantum state tomography, which deals with the reconstruction of quantum states from measurements. For large quantum systems, the exponential growth of the Hilbert space with system size renders a full reconstruction of the quantum state prohibitively demanding in terms of necessary measurements. On my poster I will present an efficient scheme for quantum state tomography using active learning and discuss its implementation. A significantly improved reconstruction is obtained when applying the active learning quantum state tomography scheme to reconstruct different multi-qubit states with varying degree of entanglement as well as to a kinetically constrained spin chain.

6. **Unraveling Quantum Scrambling with Neural Networks**

   Jan Olle

   Quantum scrambling is the process by which quantum information is spread within the degrees of freedom of many-body quantum systems. As such, understanding what are the features of a quantum system that maximise this information spreading has become a recent topic of interest of crucial importance. Graph theory provides a natural mathematical framework to encode the interactions of a quantum many-body system, and we thus employ it to study the properties of quantum scrambling as we vary the underlying graph of interactions. Predicting when a particular quantum many-body system features either strong quantum scrambling (chaotic system) or not (integrable system) is a delicate issue where sophisticated computationally expensive methods are needed. We use a graph neural network to understand better this transition and find that suprisingly simple graph-theoretic indices control this transition. In particular, we show that clustering coefficients can be used to predict its scrambling properties. While still a work in progress, we believe our results pave the way for a better understanding of how to maximize the spreading of quantum information in a controlled way.

7. **Individualized AI-ePortfolios for the entry phase in STEM degree programs (KI4TUK)**

   Stefan Küchemann

   In the first semesters of STEM studies, mathematical content particularly causes difficulties for students. Through a combination of innovative methods of educational data mining, data-based modeling, and AI, as well as theory-based didactic methods, individualized ePortfolios are created to support STEM students specifically in four competence categories relevant to study success (mathematical competence, representational competence, statistical and data literacy). These categories provide individualized information about strengths and weaknesses, and specifically identify areas for deepening and repetition. The project KI4TUK is implemented in two phases: In the first phase, data on individual student competencies is continuously collected on a web-based platform. This data consists of placement and rapid assessment tests as well as other relevant factors. Following each data collection, students are provided with learning recommendations. In the second phase, gaze data will be collected in lab courses, and then additional visual learning supports will be displayed in real time during experimentation in the field of view of the students using AR smartglasses. Both in the technical development and during the application of KI4TUK, data protection, personal rights and general principles of ethics are strictly considered. In addition to the presentation of the KI4TUK project, various initial studies will be presented in which the results indicate a significant added value of process-based measures, such as eye tracking, in AI-based prediction of learning success.

8. **Equivariance in Smoothed Particle Hydrodynamics**

   Artur Toshev

   Incorporating equivariant features into graph neural network-based learned interatomic potentials has revolutionized molecular dynamics in the last two years. At the same time, GNNs have shown to be useful on engineering data as they align well algorithmically with particle-based fluid dynamics methods. Here, we study how equivariant GNNs, specifically the SEGNN model by Brandstetter et al. 2022, improve performance on data generated using smoothed particle hydrodynamics, a Lagrangian simulation method which solves the Navier-Stokes equations on a domain discretized by particles. Unter investigation are classical 3D problems like the Reverse Poiseuille Flow discretized with a coarse resolution of 1000 points. Our preliminary results indicate that the inclusion of equivariant features results in significantly better performance, while training is 5-10x slower, and we use 2-3x more memory than simple MPNN. Finally, we discuss possible ways for scaling equivariant GNNs to larger particle systems.

9. **Field-resolved molecular fingerprinting of human blood for disease detection**

   Philip Jacob

   Human blood comprises of a complex mixture of various biofluids. In comparison to invasive clinical testing, often limited in molecular coverage and depth of analysis, infrared spectroscopy of complex biofluids provides a valuable non-invasive diagnostic approach. Recently, several studies have been undertaken to investigate the effectiveness of blood-based molecular fingerprinting using the well-established technique of Fourier transform infrared (FTIR) spectroscopy. While FTIR spectrometers are commercially available, our aim to reach new levels of sensitivity have led us to pursue the development of a new generation of ultra-short pulsed laser-based spectrometers that capture the electric field oscillations of infrared light by the process of electro-optic sampling. Few-cycle broadband mid-infrared pulses impulsively excite liquid samples in a cuvette. The sample absorbs part of the incoming radiation, and re-emits the absorbed energy subsequently in its characteristic frequency bands. The fact that the excitation pulse lasts only a few tens of femtoseconds makes it possible to temporally separate the response of the sample from the excitation. The possibility of being able to capture spectral information without being prone to the noise of the main source of radiation brings this technique to yet a new level. In combination with a novel femtosecond-laser-based spectrometer, we use linear support vector machines to train a machine-learning model that classifies healthy individuals and those affected by a disease such as cancer using information derived from blood-based electric-field molecular fingerprints. With the marriage of tools from ultrafast optics and artificial intelligence, we showcase the potential of newly devised field-resolved molecular fingerprinting as a minimally invasive, cost effective, and rapid in vitro diagnostic approach.

10. **Deep Learning for the Modeling and Inverse Design of Radiative Heat Transfer**

    Juan José García Esteban

    Deep learning is having a tremendous impact in many areas of computer science and engineering. Motivated by this success, deep neural networks are attracting increasing attention in many other disciplines, including the physical sciences. In this work, we show that artificial neural networks can be successfully used in the theoretical modeling and analysis of a variety of radiative-heat-transfer phenomena and devices. By using a set of custom-designed numerical methods able to efficiently generate the required training data sets, we demonstrate this approach in the context of three very different problems, namely (i) near-field radiative heat transfer between multilayer systems that form hyperbolic metamaterials, (ii) passive radiate cooling in photonic crystal slab structures, and (iii) thermal emission of subwavelength objects. Despite their fundamental differences in nature, in all three cases we show that simple neural-network architectures trained with data sets of moderate size can be used as fast and accurate surrogates for doing numerical simulations, as well as engines for solving inverse design and optimization in the context of radiative heat transfer. Overall, our work shows that deep learning and artificial neural networks provide a valuable and versatile toolkit for advancing the field of thermal radiation.

11. **Replacing neural networks by optimal analytical predictors for the detection of phase transitions**

    Julian Arnold

    Identifying phase transitions and classifying phases of matter is central to understanding the properties and behavior of a broad range of material systems. In recent years, machine-learning (ML) techniques have been successfully applied to perform such tasks in a data-driven manner. However, the success of this approach notwithstanding, we still lack a clear understanding of ML methods for detecting phase transitions, particularly of those that utilize neural networks (NNs). In this work, we derive analytical expressions for the optimal output of three widely used NN-based methods for detecting phase transitions. These optimal predictions correspond to the results obtained in the limit of high model capacity. Therefore, in practice they can, for example, be recovered using sufficiently large, well-trained NNs. The inner workings of the considered methods are revealed through the explicit dependence of the optimal output on the input data. By evaluating the analytical expressions, we can identify phase transitions directly from experimentally accessible data without training NNs, which makes this procedure favorable in terms of computation time. Our theoretical results are supported by extensive numerical simulations covering, e.g., topological, quantum, and many-body localization phase transitions. We expect similar analyses to provide a deeper understanding of other classification tasks in condensed matter physics.

12. **Spectroscopic evidence for engineered hadron formation in repulsive fermionic $SU(N)$ Hubbard Models**

    Miklós Antal Werner

    Particle formation represents a central theme in various branches of physics, often associated to confinement. Here we show that dynamical hadron formation can be spectroscopically detected in an ultracold atomic setting within the most paradigmatic and simplest model of condensed matter physics, the repulsive $SU(N)$ Hubbard model. By starting from an appropriately engineered initial state of the $SU(3)$ Hubbard model, not only mesons (doublons) but also baryons (trions) are naturally generated during the time evolution. In the strongly interacting limit, baryons become heavy and attract each other strongly, and their residual interaction with mesons generates meson diffusion, as captured by the evolution of the equal time density correlation function. Hadrons remain present in the long time limit, while the system thermalizes to a negative temperature state. Our conclusions extend to a large variety of initial conditions, all spatial dimensions, and for $SU(N > 2)$ Hubbard models.

13. **Predicting the Thermal Sunyaev-Zel'dovich Field using Modular and Equivariant Set-Based Neural Networks**

    Leander Thiele

    Theoretical uncertainty limits our ability to extract cosmological information from baryonic fields such as the thermal Sunyaev-Zel'dovich (tSZ) effect. Being sourced by the electron pressure field, the tSZ effect depends on baryonic physics that is usually modeled by expensive hydrodynamic simulations. We train neural networks on the IllustrisTNG-300 cosmological simulation to predict the continuous electron pressure field in galaxy clusters from gravity-only simulations. Modeling clusters is challenging for neural networks as most of the gas pressure is concentrated in a handful of voxels and even the largest hydrodynamical simulations contain only a few hundred clusters that can be used for training. Instead of conventional convolutional neural net (CNN) architectures, we choose to employ a rotationally equivariant DeepSets architecture to operate directly on the set of dark matter particles. We argue that set-based architectures provide distinct advantages over CNNs. For example, we can enforce exact rotational and permutation equivariance, incorporate existing knowledge on the tSZ field, and work with sparse fields as are standard in cosmology. We compose our architecture with separate, physically meaningful modules, making it amenable to interpretation. For example, we can separately study the influence of local and cluster-scale environment, determine that cluster triaxiality has negligible impact, and train a module that corrects for mis-centering. Our model improves by 70 % on analytic profiles fit to the same simulation data. We argue that the electron pressure field, viewed as a function of a gravity-only simulation, has inherent stochasticity, and model this property through a conditional-VAE extension to the network. This modification yields further improvement by 7 %, it is limited by our small training set however.

14. **Bubble theory: a new parametrization for classifications problems**

    Barbara Soda

    I will present a new method to parametrize the delineations of regions with different lables for classification problems in machine learning and its utility in understanding adversarial examples. The method connects algebraic and geometric mathematical objects, namely normal matrices and points and curves in a complex plane, and it could prove to be a useful tool in various fields of research.

15. **Snapshot-based analysis of quantum many-body systems with variational Monte Carlo and Neural Networks**

    Christian Manfred Reinmoser

    Microscopic descriptions of quantum many-body systems are challenging, and even with approximate theoretical descriptions at hand it can be difficult to judge how well they perform. Hence, comparing snapshots of competing theoretical approaches with experimental data is a promising application for neural networks in quantum many-body physics. In a similar fashion, we implement simple network structures to classify three different classes of numerical data for the one-dimensional t-J model: DMRG as exact numerical approach and two Monte Carlo approaches. Specifically, we use a Gutzwiller projected mean-field approach and a squeezed space approach for the Monte Carlo sampling. We are able to find which Monte Carlo approach yields snapshots more similar to the exact data. In particular, we see that the squeezed space approach snapshots are more similar to the DMRG snapshots for large values of t/J. Building on those findings, we expand our analysis to variational Monte Carlo approaches for two dimensional models.

16. **Statistical Dynamics and Linearity of Weakly Correlated Gradient Descent Based Learning**

    Ori Shem-Ur

    We characterize the gradient descent learning systems that exhibit a linear structure in the hyperparameters. We prove that linearity is equivalent to weak correlations between the first and the higher derivatives of the generalization function with respect to the hyperparameters and analyze the example of neural networks in the limit of large width. We use the equivalence between linearity and weak correlations in order to derive a bound the deviation from linearity along the study path.

17. **Towards interpretability of ANNs for spectroscopic data: inductive bias, lottery tickets, and input optimization**

    Jakub Vrabel

    The interpretability of Artificial Neural Network (ANN) –based models remains a challenging task not only for spectroscopic data. We study and compare several distinct approaches that provide an improved understanding of the model's (fully-connected network) predictions in supervised tasks and relate them to spectroscopic expertise. Namely, a weight initialization by modeled spectra and custom loss function penalization enable interpretation of the first hidden layer of the network. Additionally, lottery tickets (i.e. iteratively pruned networks) are used to reveal a local structure and positions of relevant features. The results are critically evaluated and compared to a baseline approach (feature visualization by input optimization).

18. **Bias-free evaluation of small data sets using machine-learning methods**

    Steffen Steinert

    Small data sets are a common limitation in the machine-learning based data analysis. One must be cautious not to get biased or coincidentally positive results. In this work, we identified approaches that avoid biases and can be used to determine the randomness of the result. For example, one can use a non-parametric permutation test to quantify the probability of the results generalizing to new data and test for significance. Using a repeated nested cross-validation and more than one metric for the training and the evaluation of the algorithm avoids most biases which occurred in past studies that evaluated small data sets.

19. **Unsupervised Interpretable Learning of Phases From Many-Qubit Systems**

    Nico Sadoune

    Experimental progress in qubit manufacturing calls for the development of new theoretical tools to analyze quantum data. We show how an unsupervised machine-learning technique can be used to understand short-range entangled many-qubit systems using data of local measurements. The method successfully constructs the phase diagram of a cluster-state model and detects the respective order parameters of its phases, including string order parameters. For the toric code subject to external magnetic fields, the machine identifies the explicit forms of its two stabilizers. Prior information of the underlying Hamiltonian or the quantum states is not needed; instead, the machine outputs their characteristic observables. Our work opens the door for a first-principles application of hybrid algorithms that aim at strong interpretability without supervision.

20. **Random Network Distillation for Optimal Training Data Selection**

    Samuel Tovey

    Selection of training data for machine learning applications is important part of the model training process. In most cases, training data is selected randomly and in great quantity in order to be sure that it covers the problem domain. In this poster, we demonstrate an alternative approach to selecting training data that appears to maximise model performance on a minimal dataset.

21. **Towards using Reinforcement Learning to navigate the String Flux Landscape**

    Abhishek Yogendra Dubey

    We employ the JAX framework to optimise search of vacua in the Type IIB flux landscape. The highlighting features of JAX such as auto-differentiation and just-in-time (JIT) compilation speed-up the processes considerably. Fluxes are sampled randomly and numerical algorithms are used to find the vacua. In particular, we look at the flux vacua of the Calabi-Yau hyper surface in 4 complex dimensional projective space $X_3 = CP^4_{11169}$ in large complex structure limit. The optimised process is then used in our Reinforcement Learning algorithm to learn the correlations in the flux landscape for specific models.

22. **Bloqade! An open playground for quantum simulation**

    Anna Knörr

    Quantum Monte Carlo (QMC) is a well-established general technique to simulate quantum many-body systems on classical hardware. To be efficient, it must be tailored to the specific system being studied. This poster will present the SSE formalism for QMC, how this method can be specified to the Rydberg Hamiltonian (Merali et at. 2021) and how its code implementation is being integrated into Bloqade – an open source platform for quantum simulation. This platform is being developed together with the company QuEra to supplement their expertise in quantum hardware, centered around the neutral atom architecture.

23. **Tangle of spin double helices and unconventional orders in Honeycomb Kitaev Magnets**

    Nihal Rao

    The honeycomb Kitaev-Gamma model has drawn tremendous attention due to its relevance to real Kitaev materials and its accommodation of various unconventional states of matter. Nevertheless, despite extensive studies, a little consensus is established for its phase diagram beyond the solvable Kitaev limit. Here, we utilize a combination of dierent approaches, including symmetry analysis, machine learning techniques, parallel temperature Monte Carlo and tensor network algorithms, to unravel the nature of the phases of the quantum Kitaev- model. In particular, we show that, in the most frustrated region, the system comprises modulated spin double helices with an exceptionally intricate helical pattern and anisotropic periodicity, verified by explicitly measuring the order parameter. Our results also provide a scenario to reconcile the seemingly conflicting results reported in the literature and enrich the physics of Kitaev magnetism.