

Artificial Intelligence and Machine Learning in Nuclear Physics

Amber Boehnlein, Markus Diefenthaler, Nobuo Sato, Veronique Ziegler, and Malachi Schram

*Thomas Jefferson National Accelerator Facility,
12000 Jefferson Avenue,
Newport News, Virginia,
USA*

Cristiano Fanelli

*Laboratory for Nuclear Science,
Massachusetts Institute of Technology,
Cambridge, MA 02139,
USA
The NSF AI Institute for Artificial Intelligence and Fundamental Interactions*

Morten Hjorth-Jensen

*Facility for Rare Isotope Beams and Department of Physics and Astronomy,
Michigan State University, MI 48824,
USA
Department of Physics and Center for Computing in Science Education,
University of Oslo, N-0316 Oslo,
Norway*

Tanja Horn

*Department of Physics,
The Catholic University of America,
N. E. Washington, DC 20064,
USA
Thomas Jefferson National Accelerator Facility,
12000 Jefferson Avenue,
Newport News, Virginia,
USA*

Michelle P. Kuchera

*Department of Physics and Department of Mathematics & Computer Science,
Davidson College,
North Carolina 28035,
USA*

Dean Lee, Witold Nazarewicz, and Peter Ostroumov

*Facility for Rare Isotope Beams and Department of Physics and Astronomy,
Michigan State University, MI 48824,
USA*

Kostas Orginos

*Department of Physics,
William & Mary,
Williamsburg, Virginia,
USA
Thomas Jefferson National Accelerator Facility,
12000 Jefferson Avenue,
Newport News, Virginia,
USA*

Alan Poon and Xin-Nian Wang

*Nuclear Science Division,
Lawrence Berkeley National Laboratory,
1 Cyclotron Road,
Berkeley, California 94720,
USA*

Alexander Scheinker

*Accelerator Operations and Technology Division Applied Electrodynamics Group,
Los Alamos National Laboratory,
Los Alamos, New Mexico 87544,
USA*

Michael S. Smith

*Physics Division,
Oak Ridge National Laboratory,
Oak Ridge, Tennessee, 37831-6354,
USA*

Long-Gang Pang

*Key Laboratory of Quark and Lepton Physics,
Institute of Particle Physics,
Central China Normal University, Wuhan 430079,
China*

Advances in artificial intelligence/machine learning methods provide tools that have broad applicability in scientific research. These techniques are being applied across the diversity of nuclear physics research topics, leading to advances that will facilitate scientific discoveries and societal applications. This Review gives a snapshot of nuclear physics research which has been transformed by artificial intelligence and machine learning techniques.

CONTENTS

I. Introduction	2
II. Artificial Intelligence and Machine Learning for nuclear physics in broad strokes	3
III. Areas of active research	5
A. Nuclear Theory	5
1. Low-Energy Nuclear Theory	5
2. Medium-Energy Nuclear Theory	9
3. Lattice QCD	10
4. High-Energy Nuclear Theory	12
B. Experimental Methods	14
1. Experimental Design Simulations	14
2. Streaming Detector Readout	14
3. Reconstruction and Analysis	15
C. Accelerator Science and Operations	18
1. ML-based surrogate models for accelerator models	18
2. Anomaly detection and classification	18
3. Design and control optimization	19
4. Adaptive ML for non-stationary systems	20
D. Nuclear Data	20
1. Overhauling the Nuclear Data Pipeline	20
2. Improving Compilations and Evaluations	21
3. Building Emulators and Surrogate Models	21
IV. Summary and perspectives	21
Acknowledgments	22
References	22

I. INTRODUCTION

This review represents a summary of recent work in the application of artificial intelligence (AI) and machine

learning (ML) in nuclear science, covering topics in nuclear theory, experimental methods, accelerator technology, and nuclear data. It builds on an overview of the use of AI in nuclear physics that aimed at identifying commonalities and needs (Bedaque *et al.*, 2021).

Nuclear physics is a well-established field, with more than a century of fundamental discoveries covering a huge span of degrees of freedom, energy scales and length scales, ranging from our basic understanding of fundamental constituents of matter to the structure of stars and the synthesis of the elements in the Cosmos, see Fig. 1. Experiments produce data volumes that range in complexity and heterogeneity, posing thereby enormous challenges to the design of experiments, their execution, and statistical data analysis.

Theoretical modeling of nuclear properties are, in most physical cases of interest, limited by the large amount of degrees of freedom in quantum-mechanical calculations. The analysis of experimental data and the theoretical modeling of nuclear systems aims, as is the case in all fields of physics, at uncovering the basic laws of motion in order to make predictions and estimations, as well as finding correlations and causations for strongly interacting matter. The broad aims of nuclear physics as a field corresponds to a highly distributed scientific enterprise. Experimental efforts utilize many laboratories worldwide, each with unique operation, data acquisition, and analysis methods. Similarly, the scales of focus spanned in theoretical nuclear physics lead to broad needs for algorithmic methods and uncertainty quantification. These efforts, utilizing arrays of data types across size and energy scales, creates a perfect environment for applications

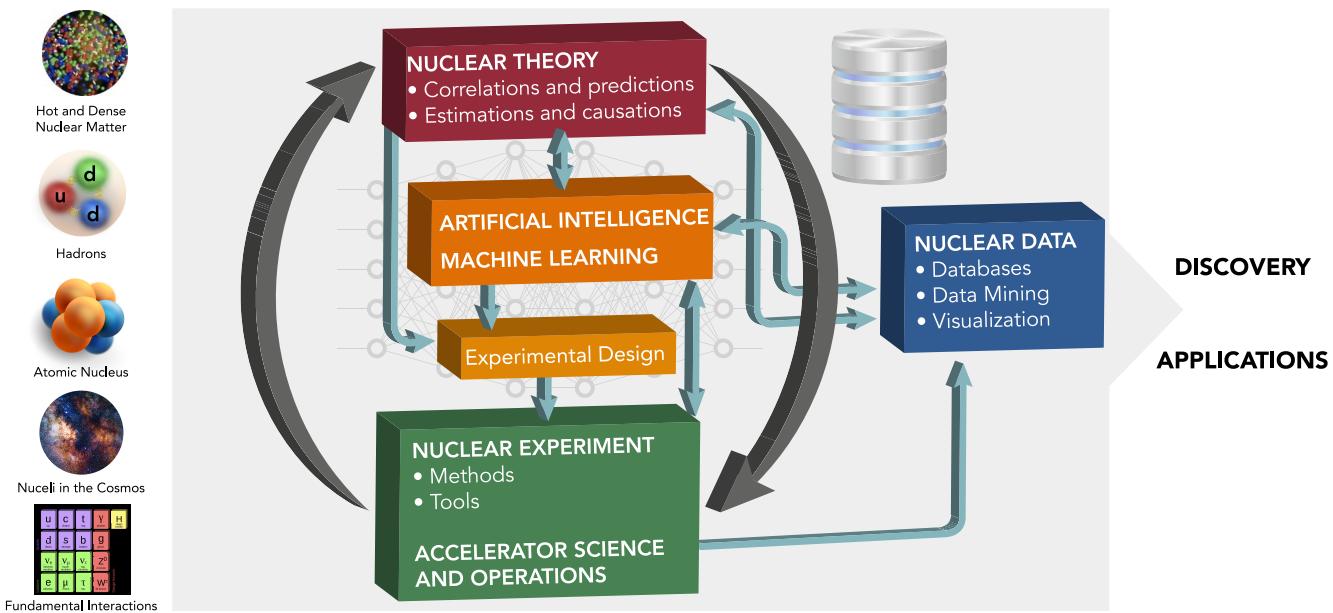


FIG. 1 Schematics relationships between the topics discussed in this review. The figure emphasizes the close connections between theory, computations (both computational science and data science as well as many elements from computer science) and experiments.

of AI/ML methods.

II. ARTIFICIAL INTELLIGENCE AND MACHINE LEARNING FOR NUCLEAR PHYSICS IN BROAD STROKES

Statistics, data science, and ML form important fields of research in modern science. They describe how to learn and make predictions from data, as well as allowing the extraction of key information about physical process and the underlying scientific laws based on large datasets. As such, recent advances in AI capabilities are being applied to advance scientific discovery in the physical sciences ([Carleo et al., 2019](#); [Deiana et al., 2021](#)).

Ideally, AI represents the science of giving computers the ability to learn without being explicitly programmed. ML tasks fall under the broader AI umbrella. The idea is that there exist generic algorithms which can be used to find patterns in a broad class of datasets without having to write code specifically for each problem. The algorithm builds its own logic based on the data. The attentive reader should however always keep in mind that machines and algorithms are to a large extent developed by humans. The insights and knowledge about a specific system plays a central role when a specific machine learning algorithm is developed.

The approaches to ML are many, but are often split into two main categories, supervised and unsupervised. In supervised learning, we have examples where we know the answer to a problem, and – based on these exam-

ples supervised learning, there are examples where the answer to a problem is known, and – based on these examples – the computer can deduce the logic behind it for future predictions. On the other hand, unsupervised learning is a method for finding patterns and relationship in datasets without any prior knowledge of the system. Many researchers also operate with a third category, namely reinforcement learning. This is a paradigm of learning inspired by behavioral psychology, where actions are learned to maximize reward. One may encounter reinforcement learning being accompanied by supervised deep learning methods. Furthermore, what is often referred to as semi-supervised learning, entails developing algorithms that aim at learning from a dataset that includes both labeled and unlabeled data.

Another way to categorize ML tasks is to consider the desired output of a system. Some of the most common tasks are ([Cranmer et al., 2021](#)):

Classification: Outputs are divided into two or more classes. The goal is to produce a model that assigns inputs into one of these classes. An example is to identify digits based on pictures of hand-written numbers.

Regression: Finding a functional relationship between an input dataset and a reference dataset. The goal is to construct a function that maps input data into continuous output values.

Clustering: Data are divided into groups with certain common traits, without knowing the different groups

beforehand. This ML task falls under the category of unsupervised learning.

Generation: Building a model to generate data that is akin to a training data set in both examples and distributions of examples. Most generative models are types of unsupervised learning.

In Table I we list many of the methods encountered in this work, with their respective abbreviations.

The methods we cover here have three main central elements in common, irrespective of whether we deal with supervised, unsupervised, or semi-supervised learning. The first element is some dataset (which can be subdivided into training, validation, and test data), the second item is a model, which is normally a function of some parameters to be determined by the chosen optimization process. The model reflects our knowledge of the system (or lack thereof). As an example, if we know that our data show a behavior similar to what would be predicted by a polynomial, fitting our data to a polynomial of some degree would determine our model.

The last part is a so-called cost (or loss, error, penalty, or risk) function which allows us to present an estimate on how good our model is in reproducing the data it is supposed to train. This is the function which is optimized in order to obtain a best prediction of the data under study. The simplest cost function in a regression analysis (fitting a continuous function to the data) is the so-called mean squared error function while for a binary classification problem, the so-called cross-entropy is widely used, see (Bishop, 2006; Hastie *et al.*, 2009; Murphy, 2012) for more details. We will refer to this part as the assessment of method in the following.

Traditionally, the field of ML has had its main focus on predictions and correlations. In ML and prediction based tasks, we are often interested in developing algorithms that are capable of learning patterns from given data in an automated fashion, and then using these learned patterns to make predictions or assessments of new data. In some cases, our primary concern is the quality of the predictions or assessments, with perhaps less focus on the underlying patterns (and probability distributions) that were learned in order to make these predictions. However, in many other nuclear physics studies, we are equally interested in being able to estimate errors and find causations. In this Colloquium, we emphasize the role of predictions and correlations as well as error estimation and causations in statistical learning and ML. For general references on these topics and discussions of frequentist and Bayesian statistics, see for example Refs. (Bishop, 2006; Goodfellow *et al.*, 2016; Hastie *et al.*, 2009; Murphy, 2012; Myren and Lawrence, 2021).

Since the aim of this Colloquium is to give an overview of present usage and research of AI and ML in nuclear physics, we utilize material from several excellent textbooks on the topic, such as the textbooks in

Refs. (Bishop, 2006; Goodfellow *et al.*, 2016; Hastie *et al.*, 2009; Murphy, 2012) and recent reviews like (Carleo *et al.*, 2019; Mehta *et al.*, 2019). We would also like to point to the theory of Bayesian Experimental Design (BED) (Chaloner and Verdinelli, 1995; Liepe *et al.*, 2013), a theory which is tailored for making optimal decisions under uncertainty.

During the last few years there has been a surge in interest in applying different ML and Bayesian methods in nuclear physics. In particular, a Bayesian approach has gained large traction since an estimation of errors plays a major role in theoretical studies, such as reliable determinations of parameters entering models for nuclear forces and density functionals. Similarly, in quantum-mechanical few- and many-body studies, a number of research groups have implemented ML based techniques in order to handle complicated correlations and degrees of freedom. These studies cover a large set of approaches, ranging from applications of deep learning methods such as ANN and restricted BM for solving the many-particle Schrödinger equation to NN in many-body methods, with the aim to learn many-body correlations. Similarly, there have been several attempts to extract information about correlations in field theory and lattice quantum chromodynamics (LQCD) from ML approaches, ranging from attempts to circumvent the fermion sign problem to learning fermion propagators and more. For recent ML applications to nuclear theory, see Sec. III.A.

In experimental nuclear physics, with increasing degrees of freedom and complexity, one faces many of the same challenges as in nuclear theory. As discussed in Sec. III.B, AI/ML approaches offer a number of optimization strategies to handle this surge in dimensionality. Many nuclear physics experiments nowadays produce terabytes or more of data, requiring the use of fast algorithms for tractable data collection and analysis. AI methods such as anomaly detection allow for exploration of data to for unforeseen phenomena. Additionally, labeled data may not be available, either due to the inability to label data or lack of knowledge of the types and behaviors of the reactions taking place. The latter are normally needed in order to generate simulated data one can use in the training process. Artificial intelligence and ML play also a considerable role in accelerator science and operations and nuclear data science, see Sections III.C and III.D, respectively.

After these more general remarks about AI and ML in nuclear physics, we move on to a description of ongoing and planned research where many of these approaches are applied to large data sets and multidimensional problems.

TABLE I Table of ML with indication on the main type of learning (S: supervised, U: unsupervised, Semi-S: semi-supervised).

Acronym	Method	Type of Learning
AE	Autoencoders	U
ANN	Artificial Neural Networks	S
BED	Bayesian Experimental Design	S
BM	Boltzmann Machines	U
BMA	Bayesian Model Averaging	S
BMM	Bayesian Model Mixing	Semi-S
BO	Bayesian Optimization	S
BNN	Bayesian Neural Networks	S
CNN	Convolutional Neural Networks	S
EMB	Ensemble Methods and Boosting, including Decision Trees and Random Forests	S
GAN	Generative Adversarial Networks	U
GP	Gaussian Processes	Semi-S
KNN	k -nearest neighbors	U
KR	Kernel Regression	S
LR	Logistic Regression	S
LSTM	Long short-term memory	S
PCA	Principal Component Analysis & Dimensionality Reduction	U
REG	Linear Regression	S
RL	Reinforcement Learning	Neither S nor U
RNN	Recurrent Neural Networks	S
SVM	Support Vector Machines	S
VAE	Variational Auto Encoders	U

III. AREAS OF ACTIVE RESEARCH

A. Nuclear Theory

1. Low-Energy Nuclear Theory

Early applications of machine learning.—In a pioneering paper, the St.Louis-Urbana collaboration (Gazula *et al.*, 1992) successfully carried out computer experiments based on ANN to study global nuclear properties across the nuclear landscape, including dripline locations, atomic masses, separation energies, and location of shell-stabilized superheavy nuclei. Their work did recognize the potential of using ML techniques to describe the variety of nuclear behavior: “*The field of nuclear physics, with a wealth of data reflecting both the fundamental principles of quantum mechanics and the behavior of strong, electromagnetic, and weak interactions on the Fermi scale of distances, offers especially fertile ground for testing and exploiting the new concept of adaptive phenomenological analysis based on neural networks.*” They concluded that “*Significant predictive ability is demonstrated, opening the prospect that neural networks may provide a valuable new tool for computing nuclear properties and, more broadly, for phenomenological description of complex many-body systems.*” Encouraged by the ability of the ANN ML technique to capture the patterns and irregularities of nuclear observables, they extended their investigations to systematics of nuclear spins and parities (Gernoth *et al.*, 1993). The SVM ML study of nuclear masses, beta-decay lifetimes, and spins/parities of nuclear ground states was reported in (Clark

and Li, 2006; Costiris *et al.*, 2008), and the application of ANN ML to beta-decays was carried out in (Costiris *et al.*, 2009).

Machine learning for data mining.—Oftentimes, it is necessary to be able to accurately calculate observables that have not been measured, to supplement the existing databases. To provide quantified interpolations and extrapolations of nuclear data, nuclear models augmented by modern ML techniques have been used. Examples include: studies of nuclear masses with EMB (Carnini and Pastore, 2020), KR (Wu *et al.*, 2021b; Wu and Zhao, 2020), and ANN (Yüksel *et al.*, 2021); calculations of the nuclear charge radii using ANN (Wu *et al.*, 2020); estimating of α -decay rates using EMB and ANN (Saxena *et al.*, 2021); constraining fission yields using mixture-density ANN (Lovell *et al.*, 2019, 2020) and BNN (Qiao *et al.*, 2021; Wang *et al.*, 2019, 2021); estimation of the total fusion cross-sections using ANN (Akkoyun, 2020); prediction of the isotopic cross-sections in proton-induced spallation reactions using BNN (Ma *et al.*, 2020a); and estimation of gamma strength functions using BO (Heim *et al.*, 2020).

Properties of heavy nuclei and nuclear density functional theory.—Kohn–Sham density functional theory (DFT) is the basic computational approach to multi-electron systems and there exists a rich literature to ML applications in the field of the electron DFT (Carleo *et al.*, 2019; Hautier *et al.*, 2010; Moreno *et al.*, 2020; Nagai *et al.*, 2020; Ryczko *et al.*, 2019; Schleder *et al.*, 2019). Nuclear DFT, rooted in the self-consistent mean-field approach (Bender *et al.*, 2003; Schunck, 2019; Yang

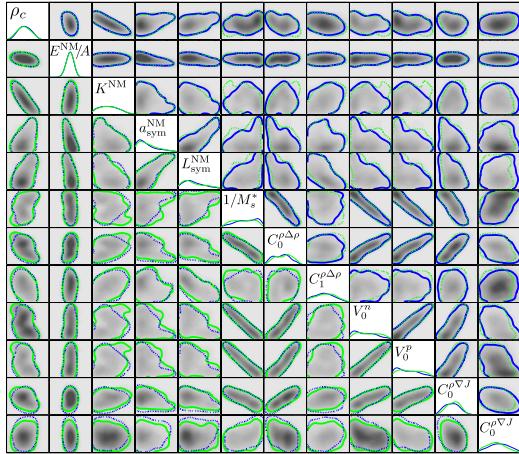


FIG. 2 Bayesian calibration of energy density functionals. Univariate and bivariate marginal estimates of the posterior distribution for the 12-dimensional parameter vector of the UNEDF1 EDF. The blue lines enclose an estimated 95% region for the posterior distribution found when only the original UNEDF1 data are accounted for; the green-outlined regions represent the same region for the posterior distribution found when the more recent mass measurements are included. Taken from (McDonnell *et al.*, 2015).

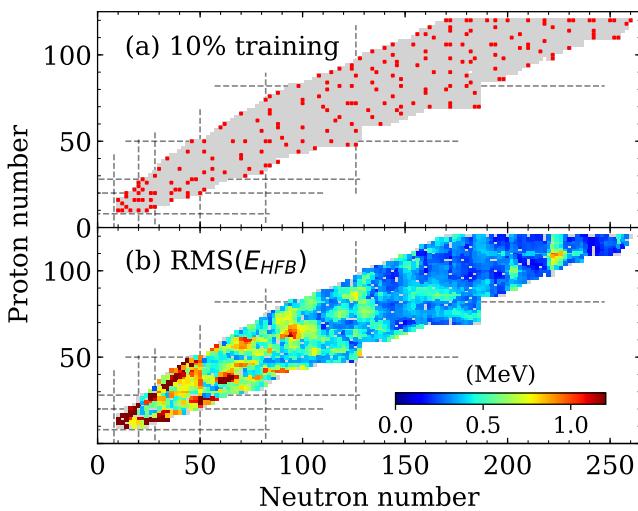


FIG. 3 DFT emulator with ANN. (a) The database nuclei (grey) as a function of N and Z . Nuclei included in the 10% training data set obtained by the active learning are marked in red. (b) The root mean square deviation between the total energy for the testing data set calculated in DFT (E_{HFB}) and with the committee of ANN. Adopted from (Lasseri *et al.*, 2020).

and Piekarewicz, 2020), is the basic computational framework for the global modeling of all nuclei, including complex exotic nuclei far from stability. An effective interaction in DFT is given by the energy density functional (EDF), whose parameters are adjusted to experimental data. Over the past decade, increasingly refined EDFs

have been developed, with increasingly complex and computationally expensive computer models, often involving BO and ANN ML (Bollapragada *et al.*, 2021; Goriely and Capote, 2014; Higdon *et al.*, 2015; Kejzlar *et al.*, 2020; McDonnell *et al.*, 2015; Navarro Pérez *et al.*, 2018; Scamps *et al.*, 2020; Schunck *et al.*, 2020a; Zhang *et al.*, 2021b). Fig. 2 shows the posterior distributions for the parameters of the UNEDF1 EDF obtained in (McDonnell *et al.*, 2015) by means of the Bayesian model calibration. These distributions have been used to provide uncertainty quantification (UQ) on UNEDF1 model predictions, in particular the r -process abundance pattern (Sprouse *et al.*, 2020), nuclear matter equation of state (Du *et al.*, 2019), and neutron star properties (Al-Mamun *et al.*, 2021).

Since global DFT computations are expensive, a promising avenue for ML applications is the emulation of DFT results (Akkoyn *et al.*, 2013; Lasseri *et al.*, 2020; Nandi *et al.*, 2021; Schunck *et al.*, 2020b). Fig. 3 shows the results of ANN calculations of (Lasseri *et al.*, 2020): a committee of ANN trained on a set of 210 nuclei is capable of predicting the ground-state and excited energies of more than 1800 atomic nuclei with significantly less computational cost than full DFT calculations.

Nuclear properties with ML.— One can improve the predictive power of a given nuclear model by comparing its predictions to existing data. Here, a powerful strategy is to estimate model residuals, i.e., deviations between experimental and calculated observables, by developing an emulator using a training set of observables taken from experiment or other theory. An emulator can be constructed by employing Bayesian approaches, such as BNN and GP. Global surveys of nuclear observables employing such a strategy can be found in (Gao *et al.*, 2021; Ma *et al.*, 2020b; Niu and Liang, 2018; Niu *et al.*, 2019a; Pastore *et al.*, 2020; Rodríguez *et al.*, 2019b; Utama and Piekarewicz, 2017, 2018; Utama *et al.*, 2016b) (extrapolations of nuclear masses with NN); (Neufcourt *et al.*, 2018; Shelley and Pastore, 2021) (extrapolations of nuclear masses with GP); (Utama *et al.*, 2016a; Wu *et al.*, 2020) (studies of nuclear radii); (Niu *et al.*, 2019b; Wu *et al.*, 2021a) (studies of beta decay rates); and (Rodríguez *et al.*, 2019a) (studies of alpha decay rates). See also (Liu *et al.*, 2021; Pastore and Carnini, 2021) for more discussion on ANN extrapolations.

By considering several global models and the most recent data one can apply the powerful techniques of Bayesian model averaging (BMA) and Bayesian model mixing (BMM) to assess model-related uncertainties in the multi-model context (Phillips *et al.*, 2021). Examples of recent model-mixed predictions using BMA include: analysis of the neutron dripline in the Ca region (Neufcourt *et al.*, 2019); studies of proton dripline and proton radioactivity (Neufcourt *et al.*, 2020a); quantifying the particle stability of nuclei (Neufcourt *et al.*, 2020b); combining models calibrated in different domains (Ke-

jzlar *et al.*, 2020); and assessing the puzzling mass of ^{80}Zr (Hamaker *et al.*, 2021). Figure 4 shows the posterior probability of existence for all nuclei in the nuclear landscape based on predictions of eleven global mass models, the most recent data on nuclear existence and masses, and three model-averaging strategies to compute the BMA weights. Figure 4 shows the posterior probability of existence for all nuclei in the nuclear landscape based on predictions of eleven global mass models, the most recent data on nuclear existence and masses, and three model-averaging strategies to compute the BMA weights.

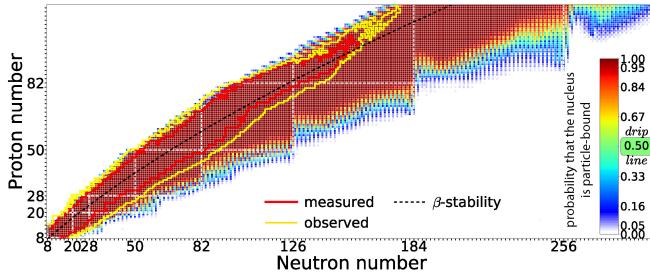


FIG. 4 Bayesian extrapolation and model averaging. The quantified landscape of nuclear existence obtained in the BMA calculations using 11 global mass models and three model-averaging strategies. For every nucleus with $Z, N \geq 8$ and $Z \leq 119$ the probability that the nucleus is bound with respect to proton and neutron decay, is marked. The domains of nuclei which have been experimentally observed and whose separation energies have been measured (and used for training) are indicated. Adopted from (Neufcourt *et al.*, 2020b).

Nuclear shell model applications— Machine Learning methods have been used to provide UQ of shell model (configuration interaction) calculations based on phenomenological two-body matrix elements. In (Yoshida *et al.*, 2018), Bayesian ML was used to compute marginal estimates of the posterior distribution for the shell-model Hamiltonian in the $0p$ space and uncertainty estimates on observables. A similar analysis, but for effective Hamiltonians in the $1s0d$ -shell, was carried out in (Fox *et al.*, 2020; Magilligan and Brown, 2020) (using PCA) and (Akkoyun *et al.*, 2021) (using ANN). Eigenvector continuation (EC) was used in (Yoshida and Shimizu, 2021) to construct an emulator of the shell-model calculations for a valence space, parameter optimization, and UQ.

Effective field theory and A-body systems.— Bayesian ML, BO, and UQ in *ab initio* nuclear theory are reviewed in (Ekström, 2020; Ekström *et al.*, 2019). There have been several studies of nucleon-nucleon scattering using Bayesian ML to estimate chiral effective field theory (EFT) truncation errors and low-energy parameters (Melendez *et al.*, 2019, 2017; Svensson *et al.*, 2021; Wesolowski *et al.*, 2019), and there have also been applications to $np \rightarrow d\gamma$ (Acharya and Bacca, 2021). In Ref. (Furnstahl *et al.*, 2020), the authors used eigenvector continuation (Frame *et al.*, 2018) as an emulator for

scattering. This is further improved in (Drischler *et al.*, 2021b) and extended to optical potentials. The application of EC as a fast emulator for uncertainty quantification for few- and many-body systems was first explored by (König *et al.*, 2020) and adapted for coupled cluster calculations and a global sensitivity analysis of ^{16}O (Ekström and Hagen, 2019) and, with Bayesian history matching (Vernon *et al.*, 2014), to global properties of ^{208}Pb (Hu *et al.*, 2021). Eigenvector continuation emulators have been used to put rigorous constraints on low-energy constants for the three-nucleon forces (Wesolowski *et al.*, 2021) and make predictions for binding of $A = 6$ nuclei (Djärv *et al.*, 2021). For other applications of eigenvector continuation, see (Eklind, 2021; Melendez *et al.*, 2021a; Sarkar and Lee, 2021; Zhang and Furnstahl, 2021). In Ref. (Connell *et al.*, 2021), the authors address whether BMA improves the extrapolation of polynomials, which are used as proxies for fixed-order EFT calculations.

Using a scattering amplitude as input data (respecting unitarity, hermiticity and analyticity), Sombillo *et al.* (Sombillo *et al.*, 2020, 2021a,b) classified the nature of the poles near threshold with multi-layer ANN. In particular, in (Sombillo *et al.*, 2020) the ANN were applied to predict the correct nature of the poles in the nucleon-nucleon scattering data from a partial wave data set. This is an example of a classification problem where the aim is to classify whether the poles represent bound, virtual or resonant states. Kaspschak *et al.* (Kaspschak and Meißner, 2021) proposed an iterative ANN perturbation theory to study s -wave scattering lengths of shallow potentials.

In Ref. (Navarro Pérez *et al.*, 2015) the statistical errors in nucleon-nucleon scattering were propagated to calculations of light nuclei. The radiative capture rate $^3\text{He} + ^4\text{He} \rightarrow ^7\text{Be} + \gamma$ was estimated with BO (Zhang *et al.*, 2020b). Bayesian ML has been applied to neutron- α scattering in chiral EFT (Kravaris *et al.*, 2020).

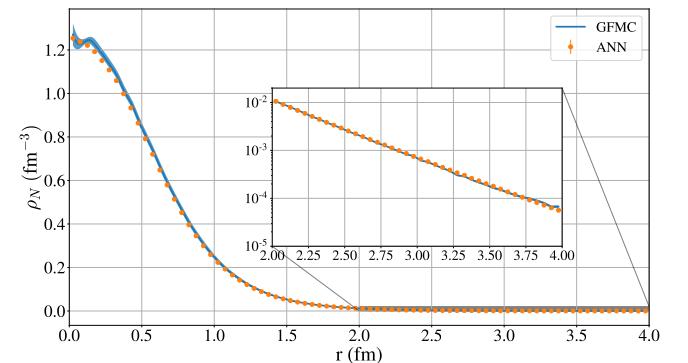


FIG. 5 Many-body variational calculations with ANN. Point-nucleon densities of ^4He for the LO pionless-EFT Hamiltonian. The solid points and the shaded area represent the ANN and Green's function Monte Carlo results, respectively. Taken from (Adams *et al.*, 2021).

In other few-body calculations, ANN were used to determine the deuteron wave function using variational optimization (Keeble and Rios, 2020). Three-body Efimov bound states were studied using ANN (Saito, 2018), and CNN were used to classify states of a quantum three-body system (Huber *et al.*, 2021). Variational Monte Carlo calculations optimized with ANN have been performed for light nuclei with up to six nucleons (Adams *et al.*, 2021; Gnech *et al.*, 2021), see Fig. 5. The latter results are interesting since the representation of the Jastrow factor in terms of ANN has the potential to introduce additional correlations. The universal approximation theorem (Bishop, 2006; Cybenko, 1989) states that ANN can represent a wide variety of non-linear functions when given appropriate weights. Overall, using ANN to extract complicated correlations in many-body calculations, seems to be a very promising approach.

In larger A -body systems, the ANN extrapolation of nuclear structure observables have been used for the no-core shell model (Negoita *et al.*, 2019), coupled cluster theory (Jiang *et al.*, 2019), and configuration interaction calculations (Yoshida, 2020). Artificial neural networks were used to learn important configurations for symmetry-adapted no-core shell-model calculations (Molchanov *et al.*, 2021). Similarly, ANN have also been used to invert Laplace transforms required to compute nuclear response functions from Euclidean time Monte Carlo data (Raghavan *et al.*, 2021). A restricted BM was used to represent many-body contact interactions using auxiliary fields (Rrapaj and Roggero, 2021). (Ismail and Gezerlis, 2021) used ML techniques to study the finite-size effects. In particular, they used ANN to extrapolate the unitary gas to the thermodynamic limit at zero range.

Another topic, which has a great potential for applications to studies of infinite matter and the Equation of State (EoS) for dense matter, is the application of ML to many-body methods like coupled cluster theory, Green's function theories, in-medium similarity renormalization group methods, etc., see, e.g., (Hjorth-Jensen *et al.*, 2017). Common to these methods is that the underlying approximations can be systematically expanded upon by including more complicated correlations. The various approaches, like for example the singles and doubles approach in coupled cluster theory (Hjorth-Jensen *et al.*, 2017), sum to infinite order so-called one-particle-one-hole and two-particle-two-hole correlations. Including three-particle correlations is computationally much more involved. Here, ML based methods can be extremely useful, in particular for studies of nuclei from calcium and beyond and infinite matter. The recent studies of (Agarwal *et al.*, 2021; Margraf and Reuter, 2018; Townsend and Vogiatzis, 2020; Wilkins *et al.*, 2019) for atomic and molecular physics systems can easily be adopted in nuclear physics, both finite nuclei and infinite matter.

Nuclear reactions.— Several aspects of UQ have been

explored in low-energy nuclear reactions. Examples include BO studies of the nucleon-nucleus optical potential (King *et al.*, 2019; Lovell *et al.*, 2021; Lovell and Nunes, 2018; Yang *et al.*, 2020) along with the sensitivity analysis (Catacora-Rios *et al.*, 2019, 2020), how BO can improve R -matrix analyses (Odell *et al.*, 2021), and statistical spatial networks used to reveal underlying patterns in nuclear reaction networks (Jiang *et al.*, 2021; Liu *et al.*, 2020).

Neutron star properties and nuclear matter equation of state (EoS)— Studies of dense nuclear matter and its pertinent EoS, with its strong implications for studies of neutron stars and studies of supernovae, is a field which has seen a considerable renaissance during the last two decades. The increased wealth of data related to cold dense matter, from laboratory experiments and theoretical simulations to neutron star observations such as the gravitational-wave events GW170817 and GW190814 (Bombaci *et al.*, 2021; Miller *et al.*, 2020), requires a framework for constraining theoretically the EoS of dense matter. Several groups have recently applied Bayesian inference, ML, and/or other statistical approaches, often combined with nuclear many-body methods, in order to properly constrain the EoS and other properties pertaining to infinite matter studies, see for example Refs. (Al-Mamum *et al.*, 2021; Ayriyan *et al.*, 2021; Brady *et al.*, 2021; Capano *et al.*, 2020; Dietrich *et al.*, 2020; Drischler *et al.*, 2020a, 2021a, 2020b; Du *et al.*, 2019; Essick *et al.*, 2021; Fujimoto *et al.*, 2021; Güven *et al.*, 2020; Han *et al.*, 2021; Kunert *et al.*, 2021; Lim and Holt, 2019; Margueron *et al.*, 2018a,b; Miller *et al.*, 2020; Morfouace *et al.*, 2019; Nätilä, J. *et al.*, 2017; Newton and Crocombe, 2021; Raaijmakers *et al.*, 2020; Tang *et al.*, 2021; Tsang *et al.*, 2019; Wang *et al.*, 2020; Xie and Li, 2020, 2021; Xu *et al.*, 2020). Several of the above references use all or large fractions of the available evidence, such as inferred masses and radii of neutron stars, estimated symmetry energies, moments of inertia, gravitational binding energies, and more.

As an example, we present in Fig. 6 the results of a Bayesian analysis by (Miller *et al.*, 2020) based on a posterior probability distribution. The figure displays the mass-radius constraints which correspond to an EoS obtained from the Bayesian analysis. Here a symmetry energy of $S = 32 \pm 2$ MeV was adopted, together with the masses of the three most massive neutron stars, the tidal deformability of GW170817 and hypothetical masses and radii to a precision of 5% and similarly a hypothetical measurement of the moment of inertia of a $1.338M_{\odot}$ star to 10% precision. The authors show that the resulting EoS is sensitive to the symmetry energy below saturation density. Better symmetry-energy estimates can then have an important consequence for our understanding of matter below saturation density. Precise neutron-star radii measurements and/or multiple tidal deformability measurements can improve our knowledge of the EoS over

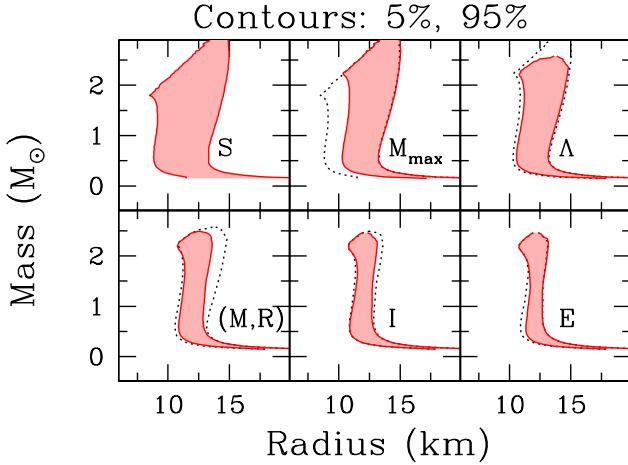


FIG. 6 Bayesian analysis of the mass-radius relation for neutron stars. The Bayesian uncertainty reflects constraints on an equation of state. Here S is the symmetry energy; M_{\max} - masses of three most massive neutron stars; Λ - tidal deformability of GW170817; (M, R) - high-precision mass-radius measurement; I - moment of inertia; and E - baryonic rest mass of a star. Taken from (Miller *et al.*, 2020).

a broader density range.

At intermediate energies, CNN have recently been applied by Zhang *et al.* (Zhang *et al.*, 2021a) to determine the impact parameters of heavy-ion collisions at low to intermediate incident energies (up to one hundred MeV/nucleon).

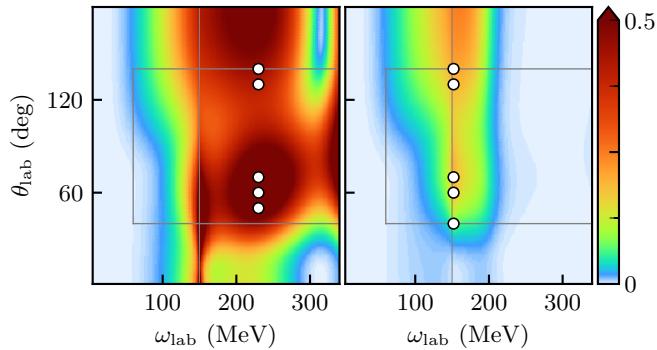


FIG. 7 BED of proton Compton scattering experiment. Shown is the expected utility of proton differential cross section measurements defined as the gain in Shannon information based on the experiment. Chiral EFT has been used to predict the functional form of the scattering amplitude. The left panel does not include EFT truncation estimates, whereas the right panel includes the EFT uncertainty. The interior box marks the experimentally accessible regime. The vertical line marks the cusp at the pion-production threshold. The white circles show the optimal five-point design kinematics. Adopted from (Melendez *et al.*, 2021b).

Experimental design, nuclear models, and ML.- Bayesian experimental design provides a general frame-

work to maximize the success of on experiment based on the best information available on the existing data, experimental conditions (including the amount of beam time available, experimental setup, budgetary constraints), and theoretical models used to process and interpret the data. The goal of BED is to maximize the expected utility of the outcome. Formally this is done by introducing the utility function that is designed by taking into account all costs and benefits (Phillips *et al.*, 2021). Recent applications of BED can be found in (Giuliani and Piekarewicz, 2021; Melendez *et al.*, 2021b). Figure 7 shows the utility function for proton Compton scattering experiment interpreted using chiral EFT. As discussed in (Melendez *et al.*, 2021b), the effect of including EFT truncation errors is significant; it shifts the region of optimal utility to lower energies. The authors of Ref. (Giuliani and Piekarewicz, 2021) used the transfer function formalism in BED of experiments, aiming at the extraction of neutron densities.

2. Medium-Energy Nuclear Theory

Nuclear femtography is an emerging field in nuclear physics that aims to map out quantum correlation functions (QCFs) that characterize the internal three-dimensional structure of nucleons and nuclei, as well as hadronization in high-energy reactions, in terms of the quark and gluon (collectively called partons) degrees of freedom of quantum chromodynamics (QCD). In contrast to any system found in Nature, the partons of QCD are not detectable experimentally due to confinement, which prevents direct access to the QCFs. Fortunately, certain classes of observables can be factorized in terms of convolutions between short-distance physics calculable in perturbative QCD and long-distance physics which is non-perturbative and encoded in the formulation of QCFs. However, in order to extract the latter, one faces an inverse problem inherited from the mathematical relation between the experimental observables and the QCFs stemming from the inability to obtain closed form solutions for the QCFs. Therefore, the only practical approach is to parameterize the QCFs and tune their associated parameters to match the data via for example Bayesian inference.

The traditional approach to implementing Bayesian inference involves the use of theory-inspired parameterizations for the QCFs, tuned via maximum likelihood estimators (Bishop, 2006; Hastie *et al.*, 2009; Murphy, 2012), along with an error analysis based on the Hessian matrix optimization (Bishop, 2006; Murphy, 2012; Pumplin *et al.*, 2002). The strategy was developed in the context of QCD global analysis of parton distribution functions (PDFs) which is a type of QCF describing the longitudinal momentum fractions of partons inside nucleons. This approach has been adopted by various groups

around the world (Accardi *et al.*, 2016; Alekhin *et al.*, 2018; Harland-Lang *et al.*, 2015; Hou *et al.*, 2021) and has found relatively good success in describing a large bank of high-energy data that are sensitive only to the one-dimensional degrees of freedom in the nucleon.

In recent years, however, Monte Carlo based methodologies for Bayesian inference (Hastie *et al.*, 2009; Mehta *et al.*, 2019; Murphy, 2012) have gained traction, providing a more reliable uncertainty quantification for QCFs in the Bayesian framework. The work of (Ball *et al.*, 2010) demonstrated the feasibility of carrying out QCD global analysis by sampling the Bayesian posterior distribution using the data resampling technique. They have also introduced neural net parameterizations to extend the flexibility for the QCF modeling and explore the degree of parameterization bias. For the case of PDFs, typically one found that in regions where the data maximally constrain the PDFs, the NN and the traditional parameterizations give qualitatively similar results, with differences becoming increasingly evident in extrapolation regions.

The Monte Carlo approach for Bayesian inference has also recently been applied to a simultaneous extraction of a variety of QCFs, including spin-dependent PDFs (Ethier *et al.*, 2017), transverse momentum distributions (Cammarota *et al.*, 2020), as well as fragmentation functions (Ethier *et al.*, 2017; Moffat *et al.*, 2021; Sato *et al.*, 2020), establishing a new paradigm in nuclear femtography. The simultaneous approach is crucial for solving the inverse problem for the QCFs, especially for those quantities that rely on each other. An example of such a situation is in semi-inclusive deep-inelastic scattering, where the experimental observables are sensitive to QCFs describing the internal structure of hadrons as well as QCFs that describe the hadronization process. In principle, each of these types of QCFs can be extracted independently from processes that are solely sensitive to each type of QCFs. However, when included within a global context, they require simultaneous analysis in order to take into account the correlations induced by uncertainties on the various interdependent QCFs themselves.

In Ref. (Ethier *et al.*, 2017), the authors showed that the strange polarization in the nucleon is mostly unconstrained if one takes fully into account the uncertainties on the spin-dependent PDFs and fragmentation functions. In Refs. (Moffat *et al.*, 2021; Sato *et al.*, 2020), a suppression of the unpolarized strange quark PDF relative to lighter quark PDFs was found to be preferred by the simultaneous extraction of spin-averaged PDFs and fragmentation functions when including the standard deep-inelastic scattering and semi-inclusive deep-inelastic scattering electromagnetic observables, semi-inclusive annihilation in e^+e^- collisions, and lepton-pair production in pp reactions. In (Cammarota *et al.*, 2020), the global analysis was performed of all existing single-spin asymmetries, providing the empirical demonstration

that the flavor-dependent nucleon tensor-charges agree within uncertainties with those computed directly in lattice QCD (LQCD).

Another new direction that has recently begun to be explored is the inclusion of LQCD data as Bayesian priors that can help overcome the difficulty in deconvoluting QCFs from experimental data. An advantage of this is that the lattice data can in principle have access into domains of the QCFs that are inaccessible experimentally or are difficult to determine due to violations of factorization in particular processes and kinematics. In Ref. (Lin *et al.*, 2018), for example, the isovector tensor charge from LQCD was used as a Bayesian prior to extract the nucleon transversity distribution. Similarly, in Ref. (Bringewatt *et al.*, 2021) the exploratory studies were carried out to include off-the-light-cone matrix elements in a QCD global analysis of spin-averaged and spin-dependent PDFs, demonstrating some level of success and/or tensions depending on the type of observables and the associated QCFs. For other studies involving LQCD, see Refs. (Del Debbio *et al.*, 2021a; Karpie *et al.*, 2019) and the following subsection. The combination of LQCD results and experimental data in the framework of Bayesian inference provide new avenues for addressing the challenges imposed by the inverse problem in QCFs and facilitate reliable comparisons between data and theory.

3. Lattice QCD

Lattice field theory is the theoretical framework for understanding the properties of strongly interacting matter. The fundamental theory of strong interactions is QCD, a quantum field theory that requires non-perturbative computations to address low energy hadronic physics. Lattice QCD provides both a rigorous definition of QCD as well as a powerful tool for numerical computations. The basic computational task in LQCD is a Monte Carlo evaluation of multi-dimensional integrals that result in the lattice regularization of QCD. Sophisticated and powerful QCD algorithms have been developed to take advantage of modern day supercomputers leading to many important results aiding experimental efforts to understand the nature of strongly interacting matter. However, despite impressive achievements, computations very close to the continuum limit that are required to reduce systematic errors are still out of reach with today's resources. Machine learning methods offer a new avenue for improving current computations as well as allowing for studies of previously impossible questions. Typical LQCD calculations proceed in two stages. First, an ensemble of gauge field configurations is generated. Subsequently, certain correlation functions of the fundamental fields are computed by averaging over the ensemble of gauge configurations. Finally, analyses of these corre-

lation functions lead to the desired physical observables (example: composite particle masses, matrix elements encoding the interaction of particles with external probes etc). Machine learning techniques are now applied to all these stages of LQCD computations promising to enhance and extend the current state of the art.

Systems at non-zero density (as in nuclear/neutron matter) or Minkowski time dynamics (parton distribution functions and transport coefficients) cannot be studied with standard Monte Carlo methods due to the fermion sign problem. Recently, it has been shown that by evaluating the relevant path integral over a field manifold deformed into complex space, the sign problem can be alleviated or even eliminated. Up to now, the choice of manifolds has been guided by either impossibly expensive calculations or (human) insight into particular models. Machine learning methods have begun to be applied, both in supervised and unsupervised learning modes (Alexandru *et al.*, 2017, 2018a,b; Bursa and Kroyter, 2018; Ohnishi *et al.*, 2019; Wynen *et al.*, 2021) to discover the integration manifolds that alleviate the sign problem and in certain cases allow for calculations previously not possible. Refinement of these methods opens an exciting new avenue for understanding QCD at non-zero density as well as understanding real-time dynamics of strongly interacting matter. At non-zero temperature the problem of reconstructing spectral functions from Euclidean correlators arises. Recently, both VAE (Chen *et al.*, 2021) and GP (Horak *et al.*, 2021) have been used to solve the associated inverse problem.

Generating gauge configuration ensembles very close to the continuum limit has also been proven a daunting computational task (Schaefer *et al.*, 2011). Present-day computations with lattice spacing below 0.05 fm are severely limited due to critical slowing down, i.e., large auto-correlation times in the Markov Chain used to generate the gauge configuration ensemble. The idea of trivializing maps (Lüscher, 2010) was introduced several years ago as a possible solution to this problem. It relied on an analytically determined map that can be used to change variables in the path integral resulting in a trivial integration weight. In (Lüscher, 2010), it was shown that such maps exist and can be constructed as solutions to a gradient flow equation whose generator can be constructed perturbatively in the flow time. Unfortunately, practical constructions of such maps have not been constructed even for simple models (Engel and Schaefer, 2011). A successful application of this program was done in the context of stochastic perturbation theory (Lüscher, 2015) which is used to perform high order perturbative computations in QCD. Machine learning methods provide a new approach in discovering these maps. In fact the idea of remapping variables with complex probability distributions to trivially distributed variables is something that is commonly done in ML. In that sense, adaptation of these methods to the context of Markov Chain Monte

Carlo (MCMC) for lattice field theory is an exciting idea with enormous potential for solving the critical slowing down problem in LQCD.

Applications of ML methods to lattice field theory calculations have already emerged. The scalar ϕ^4 theory in two dimensions is one of the first models studied, where GANs were used to reduce autocorrelation times (Pawlowski and Urban, 2020). In a work by (Albergo *et al.*, 2019; Medvidovic *et al.*, 2020), it was shown that indeed normalizing flows constructed via ANN can be trained to effectively sample the configuration space of two-dimensional scalar ϕ^4 theory up to lattice sizes of 14^2 . In (Nicoli *et al.*, 2021) thermodynamic properties of scalar ϕ^4 theory in two dimensions were studied using normalizing flows to generate field configurations confirming the efficacy of this approach. These works demonstrated that critical slowing down may be eliminated in MCMC for scalar ϕ^4 theory. However, further studies and improvements of the approach (Del Debbio *et al.*, 2021b) demonstrated that the training cost of the flow based models scales badly as the critical point is approached and the correlation length and lattice size grow, indicating that further refinements of the approach are needed for elimination of critical slowing down. The flow based methods for Monte Carlo sampling have already been extended to gauge theories (Boyda *et al.*, 2021a; Favoni *et al.*, 2020; Kanwar *et al.*, 2020; Luo *et al.*, 2020, 2021; Tomiya and Nagai, 2021), to fermionic theories (Hackett *et al.*, 2021) as well as to theories with a sign problem (Lawrence and Yamauchi, 2021). It is interesting to note that an entirely different approach in using ML methods for optimizing MCMC is the so called L2HMC approach, see (Levy *et al.*, 2018), which has been recently applied to the $U(1)$ gauge theory with fermions in (Foreman *et al.*, 2021). In this approach, ML methods are used to construct a new flow based map that replaces the Hamiltonian evolution in Hamiltonian Monte Carlo (Bishop, 2006; Li *et al.*, 2020b; Murphy, 2012). This is a promising idea that could have impact in realistic MCMC calculations in lattice field theory.

Calculations of observables in LQCD require the computation of quark propagators in the background of a large number of gauge configurations. Quark propagators are computed by solving a linear system of equations with a large and sparse coefficient matrix. Machine learning methods are used (Pederiva and Shindler, 2020) to take low precision solutions, to construct approximate observables from which full precision results are obtained via the so called all-mode-averaging technique (Shintani *et al.*, 2015), resulting in enormous increase in efficiency of the computation. Along similar lines boosted decision trees were used as approximate estimators of nucleon two and three point correlation functions used in calculations of nucleon charges and of the phase acquired by the neutron mass with a small parity violation (Yoon *et al.*, 2019). The same methodology was also employed

for correlators used in parton distribution function calculations (Zhang *et al.*, 2020a). In addition, GP was used in predicting the long distance behavior of matrix elements in PDF computations in LQCD (Alexandrou *et al.*, 2020). An interesting new idea was introduced in (Detmold *et al.*, 2021) where ML methods were used find deformations of the fields in the path integral so that the variance of observables is reduced.

Finally there is a large body of work using ML methods to understand properties of lattice field theories. These works include the prediction of lattice action parameters from field configurations (Blücher *et al.*, 2020; Shanahan *et al.*, 2018), discovering the holographic geometry in AdS/CFT descriptions of field theories (Hashimoto, 2019; Hashimoto *et al.*, 2021, 2018a,b; You *et al.*, 2018), and understanding the nature of phase transitions (Bachtis *et al.*, 2020; Blücher *et al.*, 2020; Boyda *et al.*, 2021b; Chernodub *et al.*, 2020; Wetzel and Scherzer, 2017)¹.

4. High-Energy Nuclear Theory

At extremely high temperature or density, quarks and gluons are deconfined from nucleons to form a new state of nuclear matter – the quark gluon plasma (QGP). In the early universe, this state of matter existed for about a few microseconds after the big bang and might also be at the core of some neutron stars or created during violent neutron star mergers. The field of high energy nuclear physics aims to search for its formation, the phase transition between normal nuclear matter and QGP, locate the critical point(s) and determine the deconfinement temperature in high-energy heavy-ion collisions (HIC). Many properties of QGP, such as transport coefficients (e.g., shear and bulk viscosity, conductivity and jet transport coefficient) can be extracted from experimental data using soft and hard probes.

Since the lifetime of QGP in HIC is quite short, about 10^{-23} seconds, what are detected in experiments are the relics of QGP – hadrons, photons, leptons and their momentum distributions and correlations. The properties of QGP can only be extracted indirectly through theoretical models. In practice, each observable in experimental data is entangled to many model parameters as shown in Fig. 8 which hinders the determination of a specific model parameter. Even worse, sometimes different combinations of model parameters produce degenerate output when the data are projected into low dimensions.

Two promising ML tools emerge to solve this seemingly ill-defined inverse problem. The first tool is Bayesian analysis which tends to fit all model parameters at the

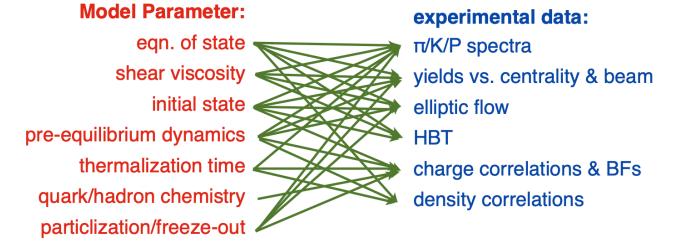


FIG. 8 Entanglement between experimental data and model parameters in determining quark gluon plasma properties, from a conference talk (Bass *et al.*, 2017).

same time using all available data. During this global fitting, if several groups of model parameters generate the same output, then the probability that the real model to be one of them decreases. On the contrary, if only one group of model parameters describes data, and changing parameters leads to large model-data differences, then the posterior distribution peaks at the optimal parameter value with small width – indicating a small model uncertainty.

Bayesian analysis is widely used in high energy nuclear physics to constrain the QCD equation of state (Pratt *et al.*, 2015), the QGP transport coefficients (Bernhard *et al.*, 2019, 2016; Paquet *et al.*, 2021), the heavy quark diffusion coefficient (Xu *et al.*, 2018), jet transport coefficient (Cao *et al.*, 2021) and the jet energy loss distributions (He *et al.*, 2019). In many applications, other ML tools are used to assist the Bayesian analysis. For example, the relativistic fluid dynamic simulations of HIC are time consuming which prevents a fast MCMC random walk in the parameter space. Emulators based on the theory of GP are employed to approximate model outputs using efficient interpolations with much fewer design points in the parameter space. Since data obtained this way are redundant and correlated, PCA is used to compress data to lower dimensions.

The observables used in Bayesian analysis are high-level features designed with personal experiences. However, feature engineering is known to be incomplete, insufficient and sometimes misleading which may lose important correlations hidden in high-dimensional data. This is unavoidable due to the high-dimensional character of the experimental data. It is difficult to recognize from exotic low-level features the non-linearly correlated patterns that are unique and robust for determining a specific model parameter.

Deep neural networks are promising ML tools to tackle the difficult inverse problem in HIC. If low-dimensional projections of model outputs are degenerate in the seemingly ill-defined inverse problem, one would expect differences still exist in high dimensions or non-linear correlations between different dimensions. The universal approximation theorem (Cybenko, 1989) ensures that

¹ Discussion of ML applications to LQCD can also be found in a recent Snowmass report (Blum *et al.*, 2021).

ANN have enough representation ability to map low-level features to some given model parameters in supervised learning. If information gets totally lost in the dynamical evolution of HIC because of entropy production, the network can never succeed in building this map. If the information of one specific model parameter survives the dynamical evolution and exists in the final output of HIC, the network has a better chance to build this map. In this sense, if the network provides high accuracy prediction in a supervised learning, it indicates that the signal does encode in the complex final state output and the network helps to decode this information. On the other hand, if the network fails, it indicates that either the information on the physical signal gets totally lost, or the used network does not have enough representation power. For the later, it is still possible with a deeper, wider or more suitable network.

The type of the nuclear phase transition is an important input to relativistic hydrodynamic simulations of HIC. At high energies, LQCD predicts that the transition between QGP and hadron resonance gas is a smooth crossover. At intermediate beam energies, it is conjectured to be a first order phase transition. Different phase transitions lead to different pressure gradients around the transition temperature which drives the QGP expansion (it also depends on the shear and bulk viscosity). In this inverse problem, one can determine the phase transition type during the dynamical evolution using final state output. Supervised CNN (Du *et al.*, 2020b; Pang *et al.*, 2018), point cloud networks (Steinheimer *et al.*, 2019), and unsupervised auto-encoders (Wang *et al.*, 2020) are trained to identify the QCD phase transition types using the final state hadrons. It is verified that signals of the phase transition survive the dynamical evolution, and deep learning succeeds in decoding this information from the final hadron distribution. To avoid overfitting to given model parameters, different parameter combinations are used to form a diverse training data set. Prediction difference analysis is used to interpret which region in the momentum space is most important for the networks to make their decisions.

Data produced in high-energy HIC are lists of particles with their four-momenta and quantum numbers. Early studies used histograms to convert this information into images which were required by two-dimensional CNN. It was found later that the point cloud network is good for this data structure (Steinheimer *et al.*, 2019). To enhance the representation power, a dynamical edge-convolution network followed by a point cloud net is used to identify self-similarity and critical fluctuations in HIC (Huang *et al.*, 2021). Figure 9 shows the architecture of the dynamical edge-convolution network. The input to the network is a list of hadrons. The output has two branches: one for event classification and the other for particle tagging. The KNN algorithm finds the k -nearest neighbors of each particle in both momentum space and feature

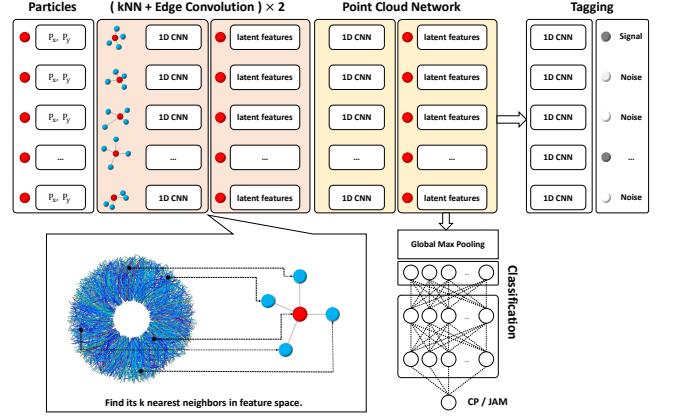


FIG. 9 **Dynamical edge-convolution neural network used for event classification and particle tagging in heavy ion collisions.** Figure taken from (Huang *et al.*, 2021).

space. Repeating the KNN and edge-convolution blocks twice helps to find long-range multi-particle correlations that are the key to searching for critical fluctuations.

The impact parameter is the transverse distance between colliding nuclei whose precise determination helps many downstream tasks. It is not possible to measure impact parameters directly through experiment. Several different ML tools are used to determine the impact parameters of HIC, including shallow neural networks (Bass *et al.*, 1996), ANN (Kuttan *et al.*, 2021; Omana Kuttan *et al.*, 2020), SVM (De Sanctis *et al.*, 2009), and EMB (Li *et al.*, 2021a, 2020a; Mallick *et al.*, 2021). In this inverse problem, data from Monte Carlo simulations are used to map final state output to the impact parameter. The traditional method uses a single observable – the particle multiplicity to determine the impact parameter. ML methods using high dimensional data result in much smaller uncertainties.

Another inverse problem associated with initial state is the nuclear structure which affects the final state output of HIC in many ways. In a prototype inverse problem, a 34-layer residual neural network is used to predict the deformation parameters of the involved nuclei (Pang *et al.*, 2019). Using the simulation data, the network succeeds in extracting the magnitude of the nuclear deformation but fails to extract the sign. The failure denotes a degeneracy raised in the dynamical process of high energy collisions. In another inverse problem, Bayesian CNN are employed to identify the 3- α and 4- α structures in the colliding light nucleus, from the final output of simulated heavy ion collisions (He *et al.*, 2021). The overall classification accuracy reaches 95% for $^{12}\text{C}/^{16}\text{O} + ^{197}\text{Au}$ collisions.

High energy jets lose energy when they traverse through hot deconfined nuclear matter. In the inverse problem, CNN are employed to predict the energy loss

ratio from final state hadrons inside a jet cone (Du *et al.*, 2020a, 2021), which allows to study the jets based on the initial energy.

The chiral magnetic effect was expected to arise from possible parity violation of strong interactions. However, all previously proposed observables suffer from large background contamination in heavy ion collisions. Deep CNN are used to identify the charge separation associated with the chiral magnetic effect (Zhao *et al.*, 2021). The network is robust to diverse conditions including different collision energies, centralities, and elliptic flow backgrounds.

Interactions between bottom and anti-bottom quarks in QGP is modeled as a heavy quark potential, whose variational function form is represented by a deep neural network (Shi *et al.*, 2021). The inputs to the network are the temperature of the QGP and the quark anti-quark separation r , the output is the heavy quark potential. Solving the pertinent differential equations numerically with this potential gives mass spectra whose difference with LQCD calculations defines the cost function. Optimizing this cost function gives the parameters of the model.

B. Experimental Methods

1. Experimental Design Simulations

Physics and detector simulations are critical for both the initial design and the optimization of complex sub-detector systems in nuclear physics experiments. These systems are usually characterized by multiple parameters capable of tuning, *e.g.*, the mechanics, the geometry, and the optics of each component.

Traditionally the global design is studied and characterized after the subsystem prototypes are ready. In the sub-detector design phase, constraints from the baseline full detector are taken into account. A well-known phenomenon observed in optimization problems with high-dimensional spaces is the so-called “curse of dimensionality” (Houle *et al.*, 2010), corresponding to a combinatorial explosion of possible values to search. Indeed, the detector design optimization can be a large combinatorial problem characterized by accurate and computationally expensive simulations performed in GEANT4 (Agostinelli *et al.*, 2003).

In this context, AI offers different optimization strategies, spanning from reinforcement learning (Sutton and Barto, 2018) to evolutionary algorithms (Deb, 2001). According to the DOE Town Halls on AI for Science (Stevens *et al.*, 2020) these new approaches can potentially “revolutionize the way experimental nuclear physics is currently done”. Among these approaches, Bayesian Optimization (BO) (Jones *et al.*, 1998; Snoek *et al.*, 2012) has gained popularity in detector design because it offers

a derivative-free principled approach to global optimization of noisy and computationally expensive black-box functions. An automated, highly-parallelized, and self-consistent procedure has been developed and tested for a dual-radiator Ring Imaging Cherenkov (d-RICH) design (Cisbani *et al.*, 2020), which has been considered as a case study. Eight main design parameters have been considered to improve the particle identification (PID) performance of the d-RICH detector (Cisbani *et al.*, 2020). Examples of design parameters are the refractive index and thickness of the aerogel radiator, the focusing mirror radius, its longitudinal and radial positions, and the three-dimensional shifts of the photon sensor tiles with respect to the mirror center on a spherical surface.

Gaussian processes have been used for regression, and a surrogate model has been reconstructed as shown in Fig. 10. These studies not only resulted in a statistically significant improvement in the PID performance compared to an existing baseline design, but they also shed light on the relevance of different features of the detector for the overall performance. Remarkably, the future Electron Ion Collider (EIC) is looking at systematically exploiting AI-based optimization strategies during the design and R&D phase of the EIC detector (Khalek *et al.*, 2021).

A pipeline based on machine learning for the LHCb electromagnetic calorimeter R&D optimization has been proposed (Boldyrev *et al.*, 2020, 2021) to evaluate its operational characteristics and determine an optimal configuration with a gain in computational time. Different cell sizes have been considered to characterize the calorimeter granularity. Signal energy deposits in the calorimeter have been studied for different background conditions by changing the number of primary vertices. Energy and spatial reconstruction were based on gradient-boosted decision trees, with the regressor trained to minimize the difference between reconstructed and generated observables, see Fig. 11. Machine Learning methods inside this pipeline are used to fine-tune the parameters of both simulation and reconstruction.

The MODE collaboration was formed to develop tools based on deep neural networks and modern automatic differentiation techniques to implement a full modeling of an experimental design, in order to achieve an end-to-end optimization. The MODE research program is summarized in (Baydin *et al.*, 2021).

2. Streaming Detector Readout

In trigger-less or streaming readout data acquisition systems, detector data is read out in continuous parallel streams that are encoded with information about when and where the data was taken. This simplifies the readout as no custom trigger hardware and firmware is needed and is beneficial for, *e.g.*, experiments that are limited by

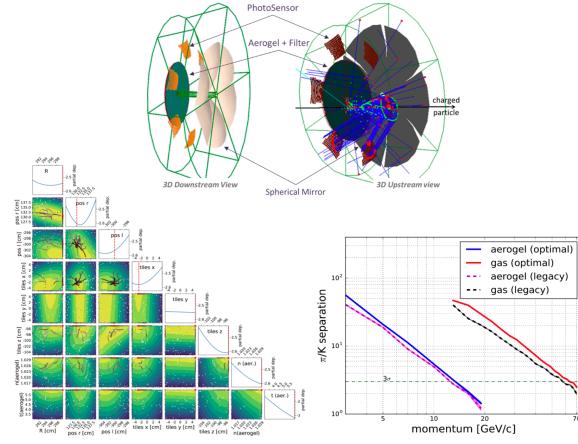


FIG. 10 (top) GEANT4 model of the d-RICH. The full 3D downstream (left) and upstream (right) views of the d-RICH detector. **(bottom left)** Surrogate model of the d-RICH design. Two-dimensional plot of the objective function used to optimize the design of the d-RICH (Cisbani *et al.*, 2020) detector. The optimization strategy involves tuning eight main design parameters characterizing the geometry and the optical properties. In order to study possible correlations, each parameter is drawn against the other. The evaluations made by the optimizer are shown through an intensity gradient in the point trail ranging from white (first call of parallel observations) to black (last call). After about 55 calls, the stopping criteria are activated. At the top of each column the partial dependence of the objective function on each variable is shown separately. **(bottom right)** Surrogate model of the d-RICH design. π/K separation as number of σ as a function of the charged particle momentum. The improvement in the separation power with the approach discussed in this paper compared to the legacy baseline design. The curves are drawn with 68% C.L. bands which are barely visible in the log plot, but this lets us better appreciate the significant difference between optimized and baseline curves. Figures taken from (Cisbani *et al.*, 2020).

event-pileup or overlapping signals from different events. Streaming readout also gives opportunity to streamline workflows for online and offline data processing and allows to take advantage AI and ML approaches.

The LHCb experiment at CERN has pioneered the idea of seamless data processing from the readout to the analysis, using software stages in early stages of the event selection. Part of this system is a custom boosted decision tree algorithm for the reconstruction of decay products of b-hadrons (Gligorov and Williams, 2013; Likhomanenko *et al.*, 2015). Progress in novel boosted decision tree algorithms allow improvements in the efficiency of decay classifications by up to 80% for high-rate events.

The CLAS12 experiment at Jefferson Lab tested a prototype streaming readout system successfully under beam conditions. The test was limited to the measurement of inclusive electroproduction of neutral pions in a lead-tungstate calorimeter and a hodoscope. An unsupervised hierarchical cluster algorithm was utilized in

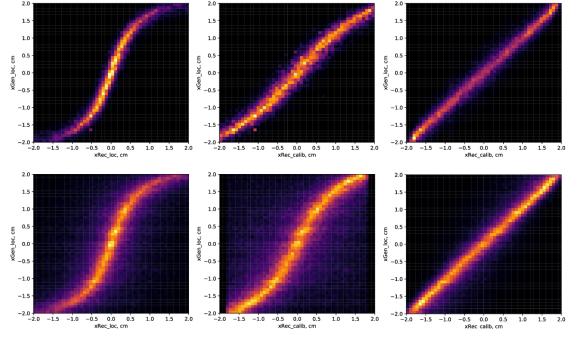


FIG. 11 Simulated calibration results for ECAL at LHCb. (left: uncalibrated) for inner modules and local coordinate x using parametric approach (centre) and XGBoost regressor (right). Top row corresponds to signal in the absence of background, bottom row to a pile-up with 10 primary vertices. Figure taken from (Boldyrev *et al.*, 2020).

real-time with real data taken in streaming readout mode to combine the time, position, and energy information at the hit level, and associate each hit with a cluster membership and an outlier score (Ameli *et al.*, 2021). The implementation based on the HDBSCAN algorithm (McInnes *et al.*, 2017) allows to successfully reject noise hits and to identify clusters for diverse topologies and large hit multiplicities.

3. Reconstruction and Analysis

Charged Particle Tracking Artificial Neural Networks provide a computational paradigm that has already been shown to meet experimental challenges at the Intensity Frontier. Deep learning approaches using neural networks have the advantage of a high level of flexibility and robustness with a minimum of assumptions about the data, which offer an effective solution to the challenges of charged particle tracking at high luminosity. At high luminosity, tracking suffers from track candidates that share hits (combinatorials). This results in hits wrongly identified as “on-track” and produces ghost tracks. In high luminosity environments the largest fraction CPU time in tracking is spent in resolving combinatorials which involves swimming in a magnetic field multiple times to find the correct candidate. Many experiments rely on a Kalman Filter method to fit tracks which involve stepping across the magnetic field to propagate the state vector and associated covariance matrix and filtering at each measurement site. This involves matrix manipulations which are CPU intensive. Therefore, the improvement in track seeding resulting from using ANN and deep learning methods, yields substantial faster track reconstruction speed. In addition the selection of the correct seed results in improved tracking efficiency (Guest *et al.*, 2018)(Gavalian *et al.*, 2020). Furthermore, noise rejection algorithms have an impact in selecting the right

combinations of hits in seeding (Komiske *et al.*, 2017a).

One of the most common deep learning algorithms employed for tracking pattern recognition are CNN. The CNN features are generally representations of the detector geometry. Machine learning algorithms used for background rejection involve topological properties of tracks to isolate signal from background(Kramárik, 2020). Outlier detection methods are used to remove noise uncorrelated hits and to classify tracks including pile-up (Ayyad *et al.*, 2018) .

Large liquid scintillator detectors can hold a large target mass for neutrino detection, for example, in solar and reactor neutrino experiments. Machine learning can benefit pure liquid scintillator detectors in event position and energy reconstruction (Qian *et al.*, 2021).

Calorimetry The GlueX experiment in Hall D at Jefferson Lab used ANN to reduce background in the GlueX forward calorimeter for the detection of photons produced in the decays of hadrons (Barsotti and Shepherd, 2020). Energy deposition characteristics in the calorimeter such as shapes, size and distribution were employed to discriminate between signal and background, where the background mostly originates from hadronic interactions that can be difficult to distinguish from low energy photon interactions. The training was done on data using ω decays. The ANN-based algorithm included in the GlueX reconstruction chain showed to be a powerful tool to reconstruct neutral particles with high efficiency and to provide substantial background rejection capability.

Particle Identification Particle identification (PID) is done with dedicated detectors capable of identifying certain particle types. For example, Cherenkov detectors are largely used in modern nuclear experiments for identifying charged particles like pions, kaons and protons corresponding to a wide range in momentum. Cherenkov detectors are typically endowed with single photon detectors and the particle type can be recognized by classifying the corresponding detected hit pattern (Fanelli, 2020). DeepRICH (Fanelli and Pomponi, 2020) is a recently developed custom architecture that combines VAE, CNN and ANN, see Fig. 12. The reconstruction performance is close to that of other established methods like FastDIRC (Hardin and Williams, 2016) with fast reconstruction times due to its implementation on GPUs that allow for parallel processing of batches of particles during the inference phase.

In (Derkach *et al.*, 2020), GANs are used to simulate the Cherenkov detector response. This architecture predicts the multidimensional distribution of the likelihood for particle identification produced by FastDIRC by-passing low-level details. Generative adversarial networks are also used in (Maevskiy *et al.*, 2020) to have a fast and accurate simulation of Cherenkov detectors; these have been trained using real data samples collected by LHCb.

The utilization of jets produced by the hadronization

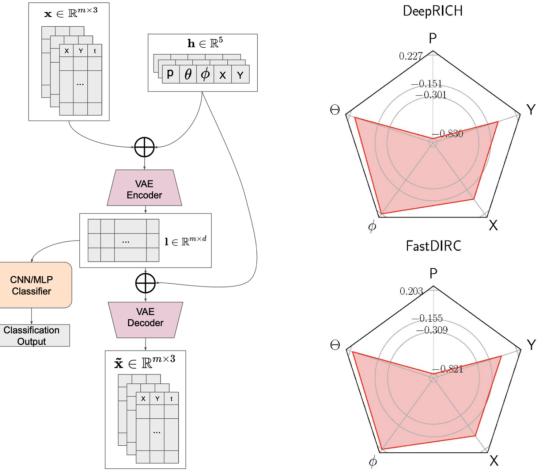


FIG. 12 (left) **A flowchart of DeepRICH:** the inputs are concatenated and fed into the encoder, which generates a set of vectors of latent variables, which are then used for both the classification of the particle and for the reconstruction of the hits. DeepRICH is a custom architecture that combines VAE, CNN and ANN. (right) Radar plots of the DIRC (Detector of Internally Reflected Cherenkov light) PID as a function of the kinematics: comparison between DeepRICH and an established reconstruction method (FastDIRC). Radar plots representing the correlation between the area under curve and each kinematics parameter for DeepRICH and FastDIRC, an established reconstruction algorithm (Hardin and Williams, 2016). These plots show that the two reconstruction algorithms perform similarly as a function of the kinematic parameters, though the first has a remarkable effective inference time per particle of $\lesssim \mu\text{s}$ when deployed on a single standard GPU. Figures taken from (Fanelli and Pomponi, 2020).

of a quark or gluon in heavy ion experiments or future electron ion colliders for nuclear physics such as EIC can be functional to a variety of fundamental topics (Page *et al.*, 2020). In (Chien, 2019), a deep CNN trained on jet images allowed the study of jet quenching utilizing quark and gluon jet substructures. Convolutional neural networks have also been used to discriminate quark and gluon jets in (Komiske *et al.*, 2017b). Different deep architectures (CNN, Dense ANN, and RNN) have been studied in (Apolinário *et al.*, 2021) for the classification of quenched jets, and in particular to discriminate between medium-like and vacuum-like jets. Identification of jets as originating from light-flavor or heavy-flavor quarks is an important aspect in inferring the nature of the particles produced in high-energy collisions. Much progress has been made in recent years on heavy-flavor tagging, with custom architectures like DeepJet (Bols *et al.*, 2020) and JetVLAD (Bielčíková *et al.*, 2021), and on strange jet tagging (Erdmann, 2020; Nakai *et al.*, 2020). Hadronic jets feature multiple tracks and extended energy deposition in both electromagnetic and hadronic calorimeters, and can represent a primary source of backgrounds for

electrons. Recent studies based on CNN showed the advantage of using low level calorimeter data represented as images in identifying electrons (Collado *et al.*, 2021). Electromagnetic showers have been classified using computer vision techniques that take advantage of lower level detector information (De Oliveira *et al.*, 2020). Bayesian neural networks have been used for the pion, kaon, and proton identification with tests done on data generated for the BES II experiment (Ye *et al.*, 2008), combining multiple features from different detectors like drift chamber, time of flight, and shower counter.

Event and Signal Classification In collision-based experiments, events are often categorized by event type for analysis. Although selection algorithms differ across experiments, the selection is typically computationally expensive in traditional analyses. In high-luminosity experiments, real-time triggers are deployed to decide which events to store for analysis. For such algorithms, fast inference speed is required. In low-energy, low luminosity collisions, such as those at rare isotope facilities, event selection post-trigger is a computational bottleneck for big data detectors such as time projection chambers (Adamson *et al.*, 2016; Bradt, 2017).

A common task in scintillator detectors in low-energy experiments is to discriminate between the neutron (n) and γ signals. Neural network analysis of pulse shapes have been shown to effectively discriminate between these signals (Doucet *et al.*, 2020).

In post-experiment analyses, deep ANN and CNN (Gavalian *et al.*, 2020; Kuchera *et al.*, 2019; Solli *et al.*, 2021) were used to classify events. Notably, seeding networks with pre-trained architectures designed for image classification allowed for fast training when events can be structured similar to images.

In low-energy neutrino experiments, artificial intelligence and machine learning techniques are typically used to differentiate different physics signal types or signals from backgrounds. One of the earliest uses of ANN to discern neutral-current from charged-current solar neutrino interactions in a heavy-water Cherenkov detector was performed by the Sudbury Neutrino Observatory experiment (Brice, 1996).

Direct kinematic measurements of tritium β decays have historically been the most sensitive to investigate the neutrino mass scale (Formaggio *et al.*, 2021). The next-generation tritium β -decay experiment Project8 plans to measure the β -electron energy spectrum via cyclotron radiation emission spectroscopy (CRES) (Montreal and Formaggio, 2009). The geometry of the detector and its electromagnetic field configuration, as well as the dynamics of the β -electrons, would give rise to different variations of the CRES signals. The collaboration is developing machine learning techniques to analyze and improve the reconstruction of these CRES events (Ashtari Esfahani *et al.*, 2020).

To answer the question of whether neutrinos are

their own antiparticles, *i.e.*, Majorana fermions, there are recently completed, operating, and planned experiments to search for neutrinoless double-beta ($0\nu\beta\beta$) decays in ^{76}Ge (Abgrall *et al.*, 2021; Agostini *et al.*, 2020; Alvis *et al.*, 2019), ^{100}Mo (Armstrong *et al.*, 2019), ^{130}Te (Anderson *et al.*, 2021; Artusa *et al.*, 2015), ^{136}Xe (Al Kharusi *et al.*, 2018; Anton *et al.*, 2019; Gando *et al.*, 2016; Gomez-Cadenas *et al.*, 2014), and other isotopes. The observation of this lepton-number-violating decay mode, in which two electrons but no neutrinos are emitted, is evidence that neutrinos are Majorana fermions. As the current limit of this decay mode is on the order of 10^{26} y, experiments — whether they are large-scale liquid scintillator detectors, semiconductor ionization detectors, cryogenic bolometers, liquid cryogenic or high-pressure gaseous time projection chambers (TPC) — are deploying machine learning techniques to distinguish and remove backgrounds in the signal search region. The “single-site” signature of $0\nu\beta\beta$ decay signal is the simultaneous appearance from the same origin of two electrons whose energies add up to the decay’s Q -value. Backgrounds tend to have “multi-site” characteristics; for example, external gamma rays that Compton-scatter at multiple locations in the detector’s active volume. A comprehensive review of $0\nu\beta\beta$ decays is found in (Dolinski *et al.*, 2019).

The use of high-purity germanium detectors (HPGe) enriched in ^{76}Ge in $0\nu\beta\beta$ -decay search has a long history (Avignone and Elliott, 2019). The GERDA experiment pioneered using ANN to identify single-site events in semi-coaxial high-purity germanium detectors (Agostini *et al.*, 2013, 2019). The use of ANN to differentiate single-site and multi-site events in HPGe was also developed in (Caldwell *et al.*, 2015; Holl *et al.*, 2019; Jany *et al.*, 2021).

The NEXT experiment exploits the topological difference between $0\nu\beta\beta$ -decay event signal and backgrounds in its ^{136}Xe high-pressure gas TPC using deep neural networks (Renner *et al.*, 2017), and specifically a convolution neural network (Kekic *et al.*, 2021) for the identification of event topology similar to that of a signal event. The DNN tools developed by NEXT have also been adapted in the conceptual design of a $^{82}\text{SeF}_6$ TPC for $0\nu\beta\beta$ -decay study (Nygren *et al.*, 2018). Another planned ^{136}Xe high-pressure gas TPC experiment PandaX-III demonstrated background suppression by two orders of magnitude in a conceptual design study (Qiao *et al.*, 2018) and an improvement of ^{136}Xe $0\nu\beta\beta$ half-life sensitivity over initial design (Li *et al.*, 2021c).

In $0\nu\beta\beta$ -decay experiments, an ample amount of the target isotope can be loaded in the scintillator, but the detector energy resolution is typically worse than other types of detectors. The KamLAND-ZEN experiment developed CNN and RNN to identify ^{10}C from cosmic-ray spallation in the liquid scintillator loaded with ^{136}Xe (Hayashida, 2019; Li *et al.*, 2019a). Efforts in

developing liquid scintillators that allow the separation of the Cherenkov light and the scintillation will facilitate machine learning to perform signal-background differentiation in $0\nu\beta\beta$ -decay experiments or other multi-purpose detectors (Askins *et al.*, 2020; Fraker, 2018; Gruszko, 2018). Large water-Cherenkov detectors could also benefit from gadolinium loading to enhance their neutron detection capability for supernova detection and searches of the diffuse supernova neutrino background (DSNB). The use of machine learning for background discrimination in such a detector has been studied (Maksimović *et al.*, 2021).

Spectroscopy Gamma-ray spectra are used, among other things, for isotope identification and fundamental nuclear structure studies. Timing resolution in high-purity germanium detectors have been optimized by fully-connected CNN architectures (Gladen *et al.*, 2020). Deep, fully-connected neural network architectures are shown to successfully identify isotopes (Abdel-Aal and Al-Haddad, 1997; Kamuda *et al.*, 2017; Medhat, 2012) and fit peaks (Abdel-Aal, 2002) in gamma spectra. Machine learning has also been shown to estimate activity levels in spectra from gamma-emitting samples (Abdel-Aal and Al-Haddad, 1997; Kamuda and Sullivan, 2018; Vigneron *et al.*, 1996). Convolutional neural networks have demonstrated robustness to spectra with unidentified background channels and calibration drifts in the detectors (Kamuda *et al.*, 2020). In addition, charged particle detection is routinely used for spectroscopy. For example, (Bailey *et al.*, 2021) uses ML to analyze signals from double sided silicon strip detectors to determine α -clustering.

C. Accelerator Science and Operations

Research in modern AI/ML techniques for accelerators is relatively new, however, it is a very active cross-cutting effort between data scientists, computer scientists, control experts, and accelerator physicists. AI/ML applications are poised to play an important role in accelerator facilities by providing data-driven digital models/twins for anomaly detection and prognostication, design optimization tools, and real time operational control/tuning. There have been explicit contributions in AI/ML for accelerators from DOE Office in Nuclear Physics (NP), however, we would be remiss to omit contributions from other programs, such DOE Office in Basic Science Energy (BES) and High Energy Physics (HEP). There have been previous efforts to document opportunities (Edelen *et al.*, 2018) and advanced control (Scheinker *et al.*, 2020a) in ML for accelerators. The following is an overview of some of these activities and new advancements since those documents.

1. ML-based surrogate models for accelerator models

Particle accelerators are complex non-linear systems that require sophisticated simulation software to capture this dynamic. Due to their complexity and evolving conditions, it's natural to explore modern data science techniques to provide surrogate models and/or a fully realized digital twin (Fuller *et al.*, 2020; Grieves and Vickers, 2017). By developing digital models, researchers are able to conduct exploratory research without impacting the physical system. The use of AI/ML to develop these digital models provides the ability to capture non-linear complex dynamics by using techniques such as Gaussian Processes Regression (Williams and Rasmussen, 1996), Quantile Regression Models (Koenker and Bassett, 1978) and RNN (Rumelhart *et al.*, 1986). These techniques can also be used to predict the future condition of the accelerator system and study anomalies, to forecast component fatigue and failures, and to optimize problems.

For simulation studies, surrogate models are the most popular examples of ML methods being used in the accelerator community to map between various accelerator parameters and beam properties at speeds that are orders of magnitude faster than computationally expensive physics models and for optimization studies (Edelen *et al.*, 2020; Emma *et al.*, 2018; Hanuka *et al.*, 2021; Kranjčević *et al.*, 2021; Li *et al.*, 2018a; Scheinker *et al.*, 2020b; Zhu *et al.*, 2021). Additionally, purely data-driven approaches have been explored to model accelerator components, such as the Fermi National Accelerator Laboratory (FNAL) booster system (John *et al.*, 2021; Kafkes and Schram, 2021).

2. Anomaly detection and classification

There is a growing amount of research in AI/ML to improve accelerator operations by detecting anomalies and classifying them. These studies explore several techniques that identify and elucidate the source of the anomalies and ultimately prevent them altogether in the future. Although it can be relatively easy to avoid these failures when they are actually happening it would be far better to avoid them all together. Unfortunately, forecasting these failures can be difficult to predict accurately with an acceptable false positive rate. Predictive diagnostics are important for improving operational efficiency, however, they can also serve as actionable precursors for control systems. There is a growing body of research in this domain, as such we present a select few recent results.

Researchers at Jefferson Lab published work on ML models for classifying C100 superconducting radio-frequency (SRF) cavity faults in the Continuous Electron Beam Accelerator Facility (CEBAF) (Solopova *et al.*, 2019; Tennant *et al.*, 2020). Traditionally, accelerator

operators are able to analyze the time-series data, identify which cavities faulted and then classify the fault type, however, manually labeling the data is laborious and time consuming. In order to accelerate the process, they developed machine learning models to identify the faulty cavity and classification fault type. The results showed that the cavity identification and fault classification models have an accuracy of 84.9% and 78.2%, respectively.

Similarly, researchers from ORNL published work on fault detection on beam loss events at the Spallation Neutron Source (SNS) facility using one pulse in advance of the actual fault (Rescic *et al.*, 2020). This work explored several machine learning techniques to predict machine failures using beam current measurements before the faults actually occurred. They evaluated these pulses using a common set of ML-based classification techniques and showed that they can identify accelerator failures prior to actually failing with almost 80% accuracy. The results were further improved by tuning the classifier parameters and using pulse properties for refining data sets leading to nearly 92% accuracy in classification of bad pulses.

In (Li *et al.*, 2021b), the authors examine the potential to predict interlocks (reflecting beam shutoff) using multiple measurements along the accelerator. Recurrence-plots based CNN (RPCNN) were used to convert the measurements into a time recurrence plots that are used as input to CNN for classification. Comparisons with EMB methods like Random Forest indicate that the performance of the random forests and RPCNN are comparable, however, the RPCNN is more successful at identifying anomalies that evolve over time.

Researchers from Jefferson Lab and ORNL have developed a novel uncertainty aware Siamese model to predict upcoming faults (Blokland *et al.*, 2021) using SNS data sets. The research combines the use of uncertainty quantification and a deep Siamese architecture to predict the similarity between beam pulses and provide an uncertainty that includes out of domain errors. The results show that this model outperforms previous results by four times in operational regions of interest. Additionally, the model performed better than previous results even for anomalies it had not seen before.

The inclusion of uncertainty quantification is an important step towards having robust and safe machine learning models for operational facilities.

3. Design and control optimization

Similar to the efforts in anomaly detection and classification, the field of accelerator optimization has recently seen advancements by applying techniques such as Bayesian optimization, generic algorithms, particle swan, and reinforcement learning. By utilizing online data from existing fast diagnostics such as beam posi-

tion monitors, beam loss monitors, and RF cavity signals, an effort has been made to develop ML-based controllers. Recent demonstrations include Bayesian methods and GP for accelerator tuning (Duris *et al.*, 2020; Hao *et al.*, 2019; Li *et al.*, 2019b; McIntire *et al.*, 2016; Shalloo *et al.*, 2020), polynomial chaos expansion-based surrogate models for uncertainty quantification (Adelmann, 2019). Particle Swarm techniques have been evaluated to optimize the tuning of aperiodic ion transport lines and for advanced particle separators (Amthor *et al.*, 2018). The use of multi-objective genetic algorithm-based (MOGA) optimization was used to minimize competing objectives steering operations of the Jefferson Lab's Continuous Electron Beam Accelerator Facility linacs (Terzić *et al.*, 2014) and showed that the dynamic heat load can be reduced by over 20% while keep the same trip rate. Additional studies using MOGA for accelerator optimization include (Li *et al.*, 2018b; Neveu *et al.*, 2019). Reinforcement learning tools have also been developed to optimize various elements of the accelerator system (Bruchon *et al.*, 2020; Gao *et al.*, 2019; Hirlaender and Bruchon, 2020; John *et al.*, 2021; Kain *et al.*, 2020; O'Shea *et al.*, 2020). Additionally, there is new research on transferring the RL policy models to FPGA to provide a low latency control response time (John *et al.*, 2021)

The accuracy of the ML methods for accelerators described above quickly degrades for systems that change with time, for which previously collected training data is no longer accurate. A major open problem faced by the ML community is the challenge of developing ML tools for complex system where the underlying dynamics is evolving (Dramsch *et al.*, 2021; Kurle *et al.*, 2019; Shimodaira, 2000; Sugiyama and Kawanabe, 2012). For systems that change very slowly with time and for which gathering large amounts of new data is feasible without interrupting operations, it is possible to utilize transfer learning techniques (Goodfellow *et al.*, 2016).

The most common transfer learning technique is update or partially re-train the model by using new data (Calandra *et al.*, 2012; Koeswiady *et al.*, 2018; Kurle *et al.*, 2019). Another transfer learning approach is domain transform in which a smaller neural networks are developed using experimental data and used as the input layer of trained ANN (Zeiler *et al.*, 2010). These transfer learning techniques can be applied to GP-based algorithms in which the prior and parameter correlations are first estimated using simulation studies and then fine-tuned with experimental data. Such transfer learning techniques have been demonstrated on a wide range of systems including cross-modal implementations (Castreronjon *et al.*, 2016) and for electron back-scatter diffraction (Shen *et al.*, 2019).

4. Adaptive ML for non-stationary systems

For accelerators in many cases new data can be acquired in real-time and used to quickly update or re-train specific layers of neural networks, however in other cases depending on what data is required repetitive re-training is not always an option. For example, if beam or accelerator characteristics change significantly diagnostics such as quadrupole magnet scan-based emittance measurements or wire-scan beam profile measurements can be time-consuming procedure that can interrupt operations. For quickly time-varying systems adaptive feedback techniques exist which are model-independent and automatically compensate for non-modeled disturbances and changes. Novel adaptive feedback algorithms have been developed to tune large groups of parameters based on noisy scalar measurements with analytic proofs of convergence and analytically known guarantees on parameter update rates, which makes them especially well-suited for particle accelerator problems (Scheinker, 2013; Scheinker and Krstić, 2017). Adaptive methods have been applied in real-time to changing accelerators to maximize FEL output power (Scheinker *et al.*, 2019), for real-time online multi-objective optimization (Scheinker *et al.*, 2020c), for non-invasive diagnostics (Scheinker and Gessner, 2015), and for online RL to learn optimal feedback control policies directly from data (Scheinker and Scheinker, 2021). A limitation of local adaptive methods is getting stuck in local minima in high dimensional parameter spaces.

Adaptive ML (AML) and continuous learning is an area of active research combining the robustness of model-independent algorithms with the global properties of ML tools such as CNN. Convolutional neural networks have been combined with adaptive feedback for fast automatic longitudinal phase space (z, E) control of time-varying electron beams (Scheinker *et al.*, 2018). The most promising AML methods tunes the low dimensional latent space of encoder-decoder type CNN based on real-time measurements and for online adjustment of inverse models that provide estimates of an accelerator’s input beam’s six-dimensional phase space distribution based only on downstream diagnostics (Scheinker, 2021; Scheinker *et al.*, 2021).

Such AML tools have the potential to enable truly autonomous accelerator controls and diagnostics that they automatically respond to non-modeled changes and disturbances in real-time and thereby keep the accelerator performance (beam energy and energy spread, beam loss, phase space quality, etc.) at a global optimal.

D. Nuclear Data

The “nuclear data pipeline” represents the interconnected steps wherein data is compiled, evaluated, pro-

cessed, and validated for end-user applications (Romano *et al.*, 2020). Evaluations, the most labor-intensive step in the pipeline, provide a recommended “best” data value (Capote *et al.*, 2010) by folding together new measurements, previous measurements, and nuclear model predictions. In some cases, it can take 5 years or more for data to pass fully through the pipeline, limited by manpower and (in some cases) outdated methodology. Machine learning has the potential to significantly improve each step of the pipeline (compilation, evaluation, processing, validation, dissemination), which may notably reduce the time lag from data measurement to incorporation into standardized databases – like the Evaluated Nuclear Data File (ENDF) (Brown *et al.*, 2018) – that are so critical for basic and applied research. Machine learning can also facilitate the creation of surrogate models or emulators that may improve the extraction of physics information from data measurements, as well as improve the predictability of evaluation models.

1. Overhauling the Nuclear Data Pipeline

Creating a new ENDF release is a time-consuming and complex process whereby the latest experimental reaction measurements, theoretical reaction calculations, theory-generated reference parameter sets, and integral and benchmark experiments are combined and adjusted in an iterative manner for optimum consistency. An effort is underway (Schnabel *et al.*, 2021, 2020) to build software “containers” to hold all of these components, as well as the current evaluations of individual reactions. By appropriately nesting and interlinking these containers to mimic portions of the nuclear data pipeline (*e.g.*, cross section measurements and models are linked together to produce an evaluation of one reaction, which is linked to other reactions to produce an evaluated library, etc.), they can be treated as interlinked nodes in a BNN. Then, GP can be used to *automatically* self-consistently update the BNN components – including the output of a new ENDF reaction data library – when *any* of the components are updated. The test cases to date utilize a sparse GP construction integrated into the BNN framework to enable modeling of energy-dependent cross sections, physics model deficiencies, and energy-dependent systematic experimental errors. This would be a completely new approach to update ENDF, and one that could be quickly adapted to incorporate new benchmark experiment types, new theory codes, and new techniques to evaluate individual reactions. When completed, this approach could be modified for use in other fields that closely interlink experiment, theory, and benchmarks.

2. Improving Compilations and Evaluations

One utilization of ML to improve evaluations is through a robust identification of outlying data points and problematic data sets. A recent example (Neudecker *et al.*, 2020) was the identification of a problematic ^{19}F neutron inelastic cross section in the ENDF database, via the use of a Random Forest regression combined with a SHapley Additive exPlanations (SHAP) feature importance metric (Lundberg and Lee, 2017) of predicted effective neutron multiplication factor k_{eff} of critical assemblies. The ML approach identified this problematic cross section that was missed with traditional validation methods; this technique may be applicable for validating other data libraries against particular features of an end-user application. Another recent study (Whewell *et al.*, 2020) focused on utilizing a variety of ML approaches, including SVM, LR, and Random Forests, to find relationships between outlying measurements and underlying details of the experiments used in an evaluation (*e.g.*, backgrounds, sample backing and impurities, detector type, incident beam type). Such an approach, which provides a robust method to reject outlying measurements and guide future experiments, was used in this specific case to improve the evaluation of the $^{239}\text{Pu}(n,\text{f})$ reaction. Random Forests were also used (Neudecker *et al.*, 2021) to combine differential data (*e.g.*, differential cross sections), application-specific integral data (*e.g.*, k_{eff} and neutron-leakage spectra from pulsed-sphere experiments), and nuclear theory to isolate likely root causes of disagreements between integral data and predictions using differential data, to select preferred differential data sets that give better agreement with integral measurements, and to specify which differential or theory developments can better reproduce integral results.

Two different ML approaches were recently combined (Bai *et al.*, 2021) to learn and reproduce the energies and widths of Giant Dipole Resonances (GDRs), which can be used to constrain ground-state deformations as well as asymmetries in the nuclear equation of state. An ANN was first used to classify nuclei into groups with one or two GDR peaks, then two multitask learning (MTL) neural nets (Zhang and Yang, 2021) were used to learn both GDR energies and widths. The MTL approach enables multiple related tasks to be learned simultaneously in a way that optimally utilizes the data for each task. As a result, the accuracy of predictions for 129 measured nuclei was doubled compared to other approaches, and then the unmeasured properties of GDRs of 79 nuclei near the β -stability line were predicted. This approach may be valuable in many evaluation approaches that require the simultaneous optimization of multiple parameters.

Uncertainty quantification (UQ) in evaluations have also been improved by learning discrepancies from existing theoretical models (Neufcourt *et al.*, 2018; Niu and Liang, 2018) and by averaging model predictions (Neuf-

court *et al.*, 2019). ML can also be used to design experiments that address nuclear data gaps for particular applications (*e.g.*, criticality experiments (Michaud *et al.*, 2019)). The new data obtained can be essential for validation efforts in the pipeline which can provide critical adjustments of evaluations.

Machine learning is also being used to help extract knowledge from published documents. Convolutional neural networks, combined with edge detection techniques, are beginning to automate the extraction of data (tables, plots, numbers) from publications (Soto, 2019). Natural language processing (NLP), widely used to process text, is an ML-enhanced textual analytics approach that is now a central ingredient of efforts to revamp numerous standardized databases; this includes extracting keywords from documents as needed for the Nuclear Science References bibliographic database (Pritychenko *et al.*, 2011). Next steps in NLP utilization in nuclear data may focus on the extraction of meaning (*i.e.*, semantics) from documents. In this approach, data and concepts could be characterized as “high value”, and certain theoretical and experimental investigations could be recommended, based on latent knowledge in the literature (Tshitoyan *et al.*, 2019).

3. Building Emulators and Surrogate Models

Phenomenological models form the foundation of many evaluation approaches, because they are computationally inexpensive and often require few input parameters. As a result, the power to extrapolate evaluations to unmeasured nuclei, to perform self-consistency checks across the nuclear chart, and to accurately capture the correlations between different nuclear properties is limited. Machine learning has the potential to dramatically improve this, by creating emulators or surrogate models that require similar computational resources as phenomenological models but capture the physics of full models. A recent example from reactor physics (Radaideh and Kozlowski, 2020) may provide a blueprint for similar advances in nuclear data. Here, deep learning ANN were used to perform UQ, sensitivity analyses, and uncertainty propagation for nuclear reactors by replacing high-fidelity reactor simulations with surrogate models.

IV. SUMMARY AND PERSPECTIVES

Artificial intelligence and machine learning techniques have in the last years gained considerable traction in scientific discovery. In particular, applications and techniques for so-called *fast* ML, *i.e.*, high-performance ML methods applied to real time experimental data processing, hold great promise for enhancing scientific discoveries in many different disciplines (Deiana *et al.*, 2021).

These developments cover a broad mix of rapidly evolving fields, from the development of ML techniques to computer and hardware architectures. For a field like nuclear physics, which covers a huge range of energy and length scales, spanning from the smallest constituents of matter to the physics of dense astronomical objects such as neutron stars, AI and ML techniques offer possibilities for new discoveries and deeper insights.

This Colloquium summarizes present and planned applications of AI and ML techniques in experimental and theoretical nuclear physics research. The vast range of scales is also reflected in new and planned nuclear physics facilities worldwide, where opportunities to incorporate AI and ML methods are expected to play an important role in the justification and design of experiments, and during the operations. In our overview, we have presented several recent experimental developments, including detector control, experimental design simulations, and accelerator operations. Furthermore, in the compilation of nuclear data, AI/ML techniques play a central role, as they do in theoretical nuclear physics. The latter field has seen an explosion in the application of AI/ML methods in the last few years. It is to be noted, however, that this Colloquium presents just a snapshot of AI in nuclear physics as of today. New AI/ML approaches are being introduced continuously at a pace difficult to keep up with. It is inevitable that over the next decades AI will play a huge role in leveraging technologies that are currently computing frontier.

Due to the broad range of scales, nuclear physics is a field where the dimensions of the problems studied quickly exceed the capabilities of traditional computational methods. Machine learning and AI offer promising paths to dimension reductions. Traditionally, many of the standard AI/ML methods focus on making predictions and finding correlations in the data sets. However, as presented in this overview, to quantify errors and find causations requires also the possibility of being able to determine models for probability distributions. Both in experiment and theory there are clear indications that statistical learning methods offer new perspectives for future research directions. Research in statistical learning techniques for both supervised and unsupervised learning, combined with for example fast ML methods and similar developments, have the potential to change the landscape of nuclear physics.

ACKNOWLEDGMENTS

The work of AB, MD, NS, MS, and VZ is supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics contract DE-AC05-06OR23177, under which Jefferson Science Associates, LLC operates the Thomas Jefferson National Accelerator Facility. NS is also supported by the U.S. Department of Energy, Of-

fice of Science, Office of Nuclear Physics in the Early Career Program. The work of CF is supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics under grant No. DE-SC0019999. The work of MHJ is supported by the U.S. Department of Energy, Office of Science, office of Nuclear Physics under grant No. DE-SC0021152 and U.S. National Science Foundation Grants No. PHY-1404159 and PHY-2013047. TH is supported by NSF grant PHY-2012430. The work of MPK is supported by the National Science Foundation under Grant No. 2012865. The work of DL is partially supported by the U.S. Department of Energy (DE-SC0013365 and DE-SC0021152) and the NUCLEI SciDAC-4 collaboration (DE-SC0018083). The work of WN is partially supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics under Award Nos. DE-SC0013365 and DE-SC0018083 (NUCLEI SciDAC-4 collaboration), and by the National Science Foundation CSSI program under award number 2004601 (BAND collaboration). KO is supported by Jefferson Science Associates, LLC under U.S. DOE Contract #DE-AC05-06OR23177, by U.S. DOE grant #DE-FG02-04ER41302, and by the Center for Nuclear Femtography grants #C2-2020-FEMT-006, #C2019-FEMT-002-05. The work of AP and XW is supported by Lawrence Berkeley National Laboratory under the U.S. Department of Energy Federal Prime Agreement DE-AC02-05CH11231. The work of AS is supported by U.S. Department of Energy (89233218CNA000001) and by the Los Alamos National Laboratory LDRD Program (Project No. 20210595DR). The work of MSS is supported by the U.S. Department of Energy, Office of Science, Office of Nuclear Physics under grant No. DE-AC05-00OR22725. The work of LGP is supported by the NSFC under grant Nos. 11861131009 and 12075098.

REFERENCES

- R. Abdel-Aal (2002), “Comparison of algorithmic and machine learning approaches for the automatic fitting of Gaussian peaks,” *Neural. Comput. Appl.* **11**, 17–29.
- R. Abdel-Aal, and M. Al-Haddad (1997), “Determination of radioisotopes in gamma-ray spectroscopy using abductive machine learning,” *Nucl. Instrum. Methods Phys. Res. A* **391** (2), 275–288.
- N. Abgrall, *et al.* (LEGEND) (2021), “The large enriched germanium experiment for neutrinoless $\beta\beta$ decay: LEGEND-1000 preconceptual design report,” [arXiv:2107.11462 \[physics.ins-det\]](https://arxiv.org/abs/2107.11462).
- A. Accardi, L. T. Brady, W. Melnitchouk, J. F. Owens, and N. Sato (2016), “Constraints on large- x parton distributions from new weak boson production and deep-inelastic scattering data,” *Phys. Rev. D* **93** (11), 114017.
- B. Acharya, and S. Bacca (2021), “Gaussian process error modeling for chiral effective-field-theory calculations of $np \leftrightarrow d\gamma$ at low energies,” [arXiv:2109.13972 \[nucl-th\]](https://arxiv.org/abs/2109.13972).
- C. Adams, G. Carleo, A. Lovato, and N. Rocco (2021), “Variational Monte Carlo calculations of $A \leq 4$ nuclei with an ar-

- tificial neural-network correlator ansatz,” *Phys. Rev. Lett.* **127**, 022502.
- P. Adamson, C. Ader, M. Andrews, N. Anfimov, I. Anghel, K. Arms, E. Arrieta-Diaz, A. Aurisano, D. Ayres, C. Backhouse, *et al.* (NOvA Collaboration) (2016), “First measurement of electron neutrino appearance in nova,” *Phys. Rev. Lett.* **116**, 151806.
- A. Adelmann (2019), “On nonintrusive uncertainty quantification and surrogate model construction in particle accelerator modeling,” *SIAM-ASA J UNCERTAIN* **7** (2), 383–416.
- V. Agarwal, S. Roy, A. Chakraborty, and R. Maitra (2021), “Accelerating coupled cluster calculations with nonlinear dynamics and supervised machine learning,” *J. Chem. Phys.* **154** (4), 044110.
- S. Agostinelli, *et al.* (2003), “Geant4—a simulation toolkit,” *Nucl. Instrum. Methods Phys. Res. A* **506** (3), 250–303.
- M. Agostini, *et al.* (2013), “Pulse shape discrimination for GERDA phase I data,” *Eur. Phys. J. C* **73** (10), 2583.
- M. Agostini, *et al.* (2019), “Probing Majorana neutrinos with double- β decay,” *Science* **365** (6460), 1445–1448.
- M. Agostini, *et al.* (GERDA) (2020), “Final results of GERDA on the search for neutrinoless double- β decay,” *Phys. Rev. Lett.* **125** (25), 252502.
- S. Akkoyun (2020), “Estimation of fusion reaction cross-sections by artificial neural networks,” *Nucl. Instrum. Methods Phys. Res. B* **462**, 51 – 54.
- S. Akkoyun, T. Bayram, S. O. Kara, and N. Yildiz (2013), “Consistent empirical physical formulas for potential energy curves of $^{38-66}\text{Ti}$ isotopes by using neural networks,” *Phys. Part. Nucl. Lett.* **10** (6), 528–534.
- S. Akkoyun, N. Laouet, and F. Benrachi (2021), “Improvement studies of an effective interaction for $N = Z$ sd-shell nuclei by neural networks,” *Bulg. J. Phys.* **48**, 1.
- S. Al Kharusi, *et al.* (nEXO) (2018), “nEXO pre-conceptual design report,” [arXiv:1805.11142 \[physics.ins-det\]](https://arxiv.org/abs/1805.11142).
- M. Al-Mamun, A. W. Steiner, J. Nättilä, J. Lange, R. O’Shaughnessy, I. Tews, S. Gandolfi, C. Heinke, and S. Han (2021), “Combining electromagnetic and gravitational-wave constraints on neutron-star masses and radii,” *Phys. Rev. Lett.* **126**, 061101.
- M. S. Albergo, G. Kanwar, and P. E. Shanahan (2019), “Flow-based generative models for Markov chain Monte Carlo in lattice field theory,” *Phys. Rev. D* **100** (3), 034515.
- S. Alekhin, J. Blümlein, and S. Moch (2018), “NLO PDFs from the ABMP16 fit,” *Eur. Phys. J. C* **78** (6), 477.
- C. Alexandrou, G. Iannelli, K. Jansen, and F. Maniago (Extended Twisted Mass) (2020), “Parton distribution functions from lattice QCD using Bayes-Gauss-Fourier transforms,” *Phys. Rev. D* **102** (9), 094508, [arXiv:2007.13800 \[hep-lat\]](https://arxiv.org/abs/2007.13800).
- A. Alexandru, P. F. Bedaque, H. Lamm, and S. Lawrence (2017), “Deep Learning Beyond Lefschetz Thimbles,” *Phys. Rev. D* **96** (9), 094505, [arXiv:1709.01971 \[hep-lat\]](https://arxiv.org/abs/1709.01971).
- A. Alexandru, P. F. Bedaque, H. Lamm, and S. Lawrence (2018a), “Finite-Density Monte Carlo Calculations on Sign-Optimized Manifolds,” *Phys. Rev. D* **97** (9), 094510.
- A. Alexandru, P. F. Bedaque, H. Lamm, S. Lawrence, and N. C. Warrington (2018b), “Fermions at Finite Density in 2+1 Dimensions with Sign-Optimized Manifolds,” *Phys. Rev. Lett.* **121** (19), 191602.
- S. I. Alvis, *et al.* (Majorana) (2019), “A search for neutrinoless double-beta decay in ^{76}Ge with 26 kg-yr of exposure from the MAJORANA DEMONSTRATOR,” *Phys. Rev. C* **100** (2), 025501.
- F. Ameli, M. Battaglieri, M. Bondi, A. Celentano, S. Boyarinov, N. Brei, T. Chiarusi, R. De Vita, C. Fanelli, V. Gyurjyan, D. Lawrence, P. Musico, C. Pellegrino, B. Raydo, and S. Vallarino (2021), “Streaming readout of the clas12 forward tagger using tridas and jana2,” [arXiv:2104.11388v1 \[physics.ins-det\]](https://arxiv.org/abs/2104.11388v1).
- A. Amthor, Z. Schillaci, D. Morrissey, M. Portillo, S. Schwarz, M. Steiner, and C. Sumithrarachchi (2018), “Experimental test of an online ion-optics optimizer,” *Nucl. Instrum. Methods Phys. Res. A* **895**, 90–99.
- M. R. Anderson, *et al.* (SNO+) (2021), “Development, characterisation, and deployment of the SNO+ liquid scintillator,” *JINST* **16** (05), P05009.
- G. Anton, *et al.* (EXO-200) (2019), “Search for neutrinoless double- β decay with the complete EXO-200 dataset,” *Phys. Rev. Lett.* **123** (16), 161802.
- L. Apolinário, N. Castro, M. C. Romão, J. Milhano, R. Pedro, and F. Peres (2021), “Deep learning for the classification of quenched jets,” [arXiv:2106.08869v1 \[hep-ph\]](https://arxiv.org/abs/2106.08869v1).
- W. R. Armstrong, *et al.* (CUPID) (2019), “CUPID pre-CDR,” [arXiv:1907.09376 \[physics.ins-det\]](https://arxiv.org/abs/1907.09376).
- D. R. Artusa, *et al.* (CUORE) (2015), “Searching for neutrinoless double-beta decay of ^{130}Te with CUORE,” *Adv. High Energy Phys.* **2015**, 879871.
- A. Ashtari Esfahani, *et al.* (Project8) (2020), “Cyclotron radiation emission spectroscopy signal classification with machine learning in Project8,” *New J. Phys.* **22** (3), 033004.
- M. Askins, *et al.* (Theia) (2020), “THEIA: an advanced optical neutrino detector,” *Eur. Phys. J. C* **80** (5), 416.
- F. T. Avignone, and S. R. Elliott (2019), “The search for double beta decay With germanium detectors: past, present, and future,” *Front. in Phys.* **7**, 6.
- A. Ayriyan, D. Blaschke, A. G. Grunfeld, D. Alvarez-Castillo, H. Grigorian, and V. Abgaryan (2021), “Bayesian analysis of multimessenger M-R data with interpolated hybrid EoS,” [arXiv:2102.13485 \[astro-ph.HE\]](https://arxiv.org/abs/2102.13485).
- Y. Ayyad, W. Mittig, D. Bazin, S. Beceiro-Novo, and M. Cortesi (2018), “Novel particle tracking algorithm based on the random sample consensus model for the Active Target Time Projection Chamber (AT-TPC),” *Nucl. Instrum. Methods Phys. Res. A* **880**, 166–173.
- D. Bachtis, G. Aarts, and B. Lucini (2020), “Mapping distinct phase transitions to a neural network,” *Phys. Rev. E* **102** (5), 053306, [arXiv:2007.00355 \[cond-mat.stat-mech\]](https://arxiv.org/abs/2007.00355).
- J. Bai, Z. Niu, B. Sun, and Y. Niu (2021), “The description of giant dipole resonance key parameters with multitask neural networks,” *Phys. Lett. B* **815**, 136147.
- S. Bailey, T. Kokalova, M. Freer, C. Wheldon, R. Smith, J. Walshe, N. Soić, L. Prepoléc, V. Tokić, F. M. Marqués, L. Achouri, F. Delaunay, M. Parlog, Q. Deshayes, B. Fernández-Dominguez, and B. Jacquot (2021), “The identification of α -clustered doorway states in $^{44,48,52}\text{Ti}$ using machine learning,” *Eur. Phys. J. A* **57** (3), 108.
- R. D. Ball, L. Del Debbio, S. Forte, A. Guffanti, J. I. Latorre, J. Rojo, and M. Ubiali (2010), “A first unbiased global NLO determination of parton distributions and their uncertainties,” *Nucl. Phys. B* **838**, 136–206.
- R. Barsotti, and M. R. Shepherd (2020), “Using machine learning to separate hadronic and electromagnetic interactions in the GlueX forward calorimeter,” arXiv e-prints , [arXiv:2002.09530 \[physics.data-an\]](https://arxiv.org/abs/2002.09530).
- S. A. Bass, J. Bernhard, and J. S. Moreland (2017), “Determination of quark-gluon-plasma parameters from

- a global Bayesian analysis,” *Nucl. Phys. A* **967**, 67–73, the 26th International Conference on Ultra-relativistic Nucleus-Nucleus Collisions: Quark Matter 2017.
- S. A. Bass, A. Bischoff, J. A. Maruhn, H. Stoecker, and W. Greiner (1996), “Neural networks for impact parameter determination,” *Phys. Rev. C* **53**, 2358–2363.
- A. G. Baydin, *et al.* (2021), “Toward Machine Learning Optimization of Experimental Design,” *Nucl. Phys. News* **31** (1), 25–28.
- P. Bedaque, A. Boehnlein, M. Cromaz, M. Diefenthaler, L. Elouadrhiri, T. Horn, M. Kuchera, D. Lawrence, D. Lee, S. Lidia, R. McKeown, W. Melnitchouk, W. Nazarewicz, K. Orginos, Y. Roblin, M. Scott Smith, M. Schram, and X.-N. Wang (2021), “A.I. for nuclear physics,” *Eur. Phys. J. A* **57** (3), 100.
- M. Bender, P.-H. Heenen, and P.-G. Reinhard (2003), “Self-consistent mean-field models for nuclear structure,” *Rev. Mod. Phys.* **75**, 121–180.
- J. E. Bernhard, J. S. Moreland, and S. A. Bass (2019), “Bayesian estimation of the specific shear and bulk viscosity of quark-gluon plasma,” *Nature Phys.* **15** (11), 1113–1117.
- J. E. Bernhard, J. S. Moreland, S. A. Bass, J. Liu, and U. Heinz (2016), “Applying Bayesian parameter estimation to relativistic heavy-ion collisions: simultaneous characterization of the initial state and quark-gluon plasma medium,” *Phys. Rev. C* **94** (2), 024907.
- J. Bielčíková, R. K. Elayavalli, G. Ponimakin, J. H. Putschke, and J. Sivic (2021), “Identifying heavy-flavor jets using vectors of locally aggregated descriptors,” *J. Instrum.* **16** (03), P03017.
- C. M. Bishop (2006), *Pattern Recognition and Machine Learning* (Springer Verlag, Berlin).
- W. Blokland, M. Schram, K. Rajput, P. Ramuhalli, C. Peters, Y. Yucesan, A. Zhukov, and T. Jeske (2021), “Uncertainty aware anomaly detection to predict errant beam pulses in the sns accelerator,” [arXiv:2110.12006 \[physics.acc-ph\]](https://arxiv.org/abs/2110.12006).
- S. Blücher, L. Kades, J. M. Pawłowski, N. Strodthoff, and J. M. Urban (2020), “Towards novel insights in lattice field theory with explainable machine learning,” *Phys. Rev. D* **101** (9), 094507, [arXiv:2003.01504 \[hep-lat\]](https://arxiv.org/abs/2003.01504).
- T. Blum, P. Boyle, T. Izubuchi, L. Jin, C. Jung, C. Lehner, M. Lin, Lin, and A. Tomiya (2021), https://www.snowmass21.org/docs/files/summaries/CompF/SNOWMASS21-CompF3_CompF2-TF5_TF0_Akio_Tomiya-131.pdf.
- A. Boldyrev, D. Derkach, F. Ratnikov, and A. Shevelev (2020), “ML-assisted versatile approach to Calorimeter R&D,” *J. Instrum.* **15** (09), C09030.
- A. Boldyrev, D. Derkach, F. Ratnikov, and A. Shevelev (2021), “Machine Learning in Calorimeter optimization,” in *J. Phys. Conf. Ser.*, Vol. 1740 (IOP Publishing) p. 012047.
- R. Bollapragada, M. Menickelly, W. Nazarewicz, J. O’Neal, P.-G. Reinhard, and S. M. Wild (2021), “Optimization and supervised machine learning methods for fitting numerical physics models without derivatives,” *J. Phys. G* **48** (2), 024001.
- E. Bols, J. Kieseler, M. Verzetti, M. Stoye, and A. Stakia (2020), “Jet flavour classification using deepjet,” *J. Instrum.* **15** (12), P12012.
- I. Bombaci, A. Drago, D. Logoteta, G. Pagliara, and I. Vidaña (2021), “Was GW190814 a black hole–strange quark star system?” *Phys. Rev. Lett.* **126**, 162702.
- D. Boyda, G. Kanwar, S. Racanière, D. J. Rezende, M. S. Albergo, K. Cranmer, D. C. Hackett, and P. E. Shanahan (2021a), “Sampling using $SU(N)$ gauge equivariant flows,” *Phys. Rev. D* **103** (7), 074504, [arXiv:2008.05456 \[hep-lat\]](https://arxiv.org/abs/2008.05456).
- D. L. Boyda, M. N. Chernodub, N. V. Gerasimeniuk, V. A. Goy, S. D. Liubimov, and A. V. Molochkov (2021b), “Finding the deconfinement temperature in lattice Yang-Mills theories from outside the scaling window with machine learning,” *Phys. Rev. D* **103** (1), 014509, [arXiv:2009.10971 \[hep-lat\]](https://arxiv.org/abs/2009.10971).
- J. W. Bradt (2017), *Measurement of isobaric analogue resonances of ^{47}Ar with the active target time projection chamber*, Ph.D. thesis (Michigan State University).
- J. Brady, P. Wen, and J. W. Holt (2021), “Normalizing flows for microscopic many-body calculations: An application to the nuclear equation of state,” *Phys. Rev. Lett.* **127**, 062701.
- S. J. Brice (1996), *Monte carlo and analysis techniques for the Sudbury Neutrino Observatory*, Phd thesis (University of Oxford).
- J. Bringewatt, N. Sato, W. Melnitchouk, J.-W. Qiu, F. Stevens, and M. Constantinou (2021), “Confronting lattice parton distributions with global QCD analysis,” *Phys. Rev. D* **103** (1), 016003.
- D. Brown, *et al.* (2018), “ENDF/B-VIII.0: the 8th major release of the nuclear reaction data library with CIELO-project cross sections, new standards and thermal scattering data,” *Nucl. Data Sheets* **148**, 1–142.
- N. Bruchon, G. Fenu, G. Gaio, M. Lonza, F. H. O’Shea, F. A. Pellegrino, and E. Salvato (2020), “Basic reinforcement learning techniques to control the intensity of a seeded free-electron laser,” *Electronics* **9** (5), 781.
- F. Bursa, and M. Kroyter (2018), “A simple approach towards the sign problem using path optimisation,” *JHEP* **12**, 054.
- R. Calandra, T. Raiko, M. P. Deisenroth, and F. M. Pouzols (2012), “Learning deep belief networks from non-stationary streams,” in *Proc. Int. Conf. Artificial Neural Netw.* (Springer) pp. 379–386.
- A. Caldwell, F. Cossavella, B. Majorovits, D. Palioselitis, and O. Volynets (2015), “Signal recognition efficiencies of artificial neural-network pulse-shape discrimination in HPGe $0\nu\beta\beta$ -decay searches,” *Eur. Phys. J. C* **75** (7), 350.
- J. Cammarota, L. Gamberg, Z.-B. Kang, J. A. Miller, D. Pitonyak, A. Prokudin, T. C. Rogers, and N. Sato (Jefferson Lab Angular Momentum) (2020), “Origin of single transverse-spin asymmetries in high-energy collisions,” *Phys. Rev. D* **102** (5), 054002.
- S. Cao, *et al.* (JETSCAPE) (2021), “Determining the jet transport coefficient \hat{q} from inclusive hadron suppression measurements using Bayesian parameter estimation,” *Phys. Rev. C* **104** (2), 024905.
- C. D. Capano, I. Tews, S. M. Brown, B. Margalit, S. De, S. Kumar, D. A. Brown, B. Krishnan, and S. Reddy (2020), “Stringent constraints on neutron-star radii from multimesenger observations and nuclear theory,” *Nat. Astron.* **4** (6), 625–632.
- R. Capote, D. L. Smith, and A. Trkov (2010), “Nuclear data evaluation methodology including estimates of covariances,” *EPJ Web of Conferences* **8**, 04001.
- G. Carleo, I. Cirac, K. Cranmer, L. Daudet, M. Schuld, N. Tishby, L. Vogt-Maranto, and L. Zdeborová (2019), “Machine learning and the physical sciences,” *Rev. Mod. Phys.* **91**, 045002.

- M. Carnini, and A. Pastore (2020), “Trees and forests in nuclear physics,” *J. Phys. G* **47** (8), 082001.
- L. Castrejon, Y. Aytar, C. Vondrick, H. Pirsiavash, and A. Torralba (2016), “Learning aligned cross-modal representations from weakly aligned data,” in *Proc. IEEE Computer Vision and Pattern Recognition Conf.*, pp. 2940–2949.
- M. Catacora-Rios, G. B. King, A. E. Lovell, and F. M. Nunes (2019), “Exploring experimental conditions to reduce uncertainties in the optical potential,” *Phys. Rev. C* **100** (6), 064615.
- M. Catacora-Rios, G. B. King, A. E. Lovell, and F. M. Nunes (2020), “Which observable offers better constraints on the optical potential?” [arXiv:2012.06653 \[nucl-th\]](#).
- B. c. v. Terzić, A. S. Hofler, C. J. Reeves, S. A. Khan, G. A. Krafft, J. Benesch, A. Freyberger, and D. Ranjan (2014), “Simultaneous optimization of the cavity heat load and trip rates in linacs using a genetic algorithm,” *Phys. Rev. ST Accel. Beams* **17**, 101003.
- K. Chaloner, and I. Verdinelli (1995), “Bayesian experimental design: A review,” *Stat. Sci.* **10** (3), 273–304.
- S. Y. Chen, H. T. Ding, F. Y. Liu, G. Papp, and C. B. Yang (2021), “Machine learning spectral functions in lattice QCD,” [arXiv:2110.13521 \[hep-lat\]](#).
- M. N. Chernodub, H. Erbin, V. A. Goy, and A. V. Molochkov (2020), “Topological defects and confinement with machine learning: the case of monopoles in compact electrodynamics,” *Phys. Rev. D* **102** (5), 054501, [arXiv:2006.09113 \[hep-lat\]](#).
- Y.-T. Chien (2019), “Probing heavy ion collisions using quark and gluon jet substructure with machine learning,” *Nucl. Phys. A* **982**, 619–622.
- E. Cisbani, *et al.* (2020), “AI-optimized detector design for the future electron-ion collider: the dual-radiator RICH case,” *J. Instrum.* **15** (05), P05009–P05009.
- J. W. Clark, and H. Li (2006), “Application of support vector machines to global prediction of nuclear properties,” *Int. J. Mod. Phys. B* **20**, 5015–5029.
- J. Collado, J. N. Howard, T. Faucett, T. Tong, P. Baldi, and D. Whiteson (2021), “Learning to identify electrons,” *Phys. Rev. D* **103** (11), 116028.
- M. A. Connell, I. Billig, and D. R. Phillips (2021), “Does Bayesian model averaging improve polynomial extrapolations? Two toy problems as tests,” *J. Phys. G* **48** (10), 104001.
- N. Costiris, E. Mavrommatis, K. Gernoth, and J. Clark (2009), “Decoding Beta-Decay Systematics: A Global Statistical Model for Beta-Halfives,” *Phys. Rev. C* **80**, 044332.
- N. J. Costiris, E. Mavrommatis, K. A. Gernoth, J. W. Clark, and H. Li (2008), “Statistical global modeling of beta-decay halfives systematics using multilayer feedforward neural networks and support vector machines,” in *17th Symposium of the Hellenic Nuclear Physics Society on Nuclear Physics, Ioannina, Greece, May 30-31, 2008*.
- K. Cranmer, U. Seljak, and K. Terao (2021), “Machine Learning,” *Prog. Theor. Exp. Phys.* .
- G. Cybenko (1989), “Approximation by superpositions of a sigmoidal function,” *Math. Control Signals Syst.* **2**, 303.
- L. De Oliveira, B. Nachman, and M. Paganini (2020), “Electromagnetic showers beyond shower shapes,” *Nucl. Instrum. Methods Phys. Res. A* **951**, 162879.
- J. De Sanctis, M. Masotti, M. Bruno, M. D’Agostino, E. Geraci, G. Vannini, and A. Bonasera (2009), “Classification of the impact parameter in nucleus-nucleus collisions by a support vector machine method,” *J. Phys. G* **36**, 015101.
- K. Deb (2001), *Multi-objective optimization using evolutionary algorithms*, Vol. 16 (John Wiley & Sons).
- A. M. Deiana, *et al.* (2021), “Applications and techniques for fast machine learning in science,” [arXiv:2110.13041 \[cs.LG\]](#).
- L. Del Debbio, T. Giani, J. Karpie, K. Orginos, A. Radyushkin, and S. Zafeiropoulos (2021a), “Neural-network analysis of Parton Distribution Functions from Ioffe-time pseudodistributions,” *JHEP* **02**, 138.
- L. Del Debbio, J. Marsh Rossney, and M. Wilson (2021b), “Efficient modeling of trivializing maps for lattice ϕ^4 theory using normalizing flows: A first look at scalability,” *Phys. Rev. D* **104**, 094507.
- D. Derkach, N. Kazeev, F. Ratnikov, A. Ustyuzhanin, and A. Volokhova (2020), “Cherenkov detectors fast simulation using neural networks,” *Nucl. Instrum. Methods Phys. Res. A* **952**, 161804.
- W. Detmold, G. Kanwar, H. Lamm, M. L. Wagman, and N. C. Warrington (2021), “Path integral contour deformations for observables in $SU(N)$ gauge theory,” *Phys. Rev. D* **103** (9), 094517, [arXiv:2101.12668 \[hep-lat\]](#).
- T. Dietrich, M. W. Coughlin, P. T. H. Pang, M. Bulla, J. Heinzel, L. Issa, I. Tews, and S. Antier (2020), “Multi-messenger constraints on the neutron-star equation of state and the Hubble constant,” *Science* **370** (6523), 1450–1453.
- T. Djärv, A. Ekström, C. Forssén, and H. T. Johansson (2021), “Fast & rigorous predictions for $A = 6$ nuclei with Bayesian posterior sampling,” [arXiv:2108.13313 \[nucl-th\]](#).
- M. J. Dolinski, A. W. P. Poon, and W. Rodejohann (2019), “Neutrinoless double-beta decay: status and prospects,” *Ann. Rev. Nucl. Part. Sci.* **69**, 219–251.
- E. Doucet, T. Brown, P. Chowdhury, C. Lister, C. Morse, P. Bender, and A. Rogers (2020), “Machine learning n/γ discrimination in CLYC scintillators,” *Nucl. Instrum. Methods Phys. Res. A* **954**, 161201.
- J. S. Dramsch, M. Lüthje, and A. N. Christensen (2021), “Complex-valued neural networks for machine learning on non-stationary physical data,” *Computers & Geosciences* **146**, 104643.
- C. Drischler, R. J. Furnstahl, J. A. Melendez, and D. R. Phillips (2020a), “How well do we know the neutron-matter equation of state at the densities inside neutron stars? A Bayesian approach with correlated uncertainties,” *Phys. Rev. Lett.* **125**, 202702.
- C. Drischler, S. Han, and S. Reddy (2021a), “Large and massive neutron stars: Implications for the sound speed in dense QCD,” [arXiv:2110.14896 \[nucl-th\]](#).
- C. Drischler, J. A. Melendez, R. J. Furnstahl, and D. R. Phillips (2020b), “Quantifying uncertainties and correlations in the nuclear-matter equation of state,” *Phys. Rev. C* **102**, 054315.
- C. Drischler, M. Quinonez, P. Giuliani, A. Lovell, and F. Nunes (2021b), “Toward emulating nuclear reactions using eigenvector continuation,” *Phys. Lett. B* , 136777.
- X. Du, A. W. Steiner, and J. W. Holt (2019), “Hot and dense homogeneous nucleonic matter constrained by observations, experiment, and theory,” *Phys. Rev. C* **99**, 025803.
- Y.-L. Du, D. Pablos, and K. Tywoniuk (2020a), “Deep learning jet modifications in heavy-ion collisions,” *JHEP* **21**, 206.
- Y.-L. Du, D. Pablos, and K. Tywoniuk (2021), “Jet to-

- mography in heavy ion collisions with deep learning," arXiv:2106.11271 [hep-ph].
- Y.-L. Du, K. Zhou, J. Steinheimer, L.-G. Pang, A. Motorinenko, H.-S. Zong, X.-N. Wang, and H. Stöcker (2020b), "Identifying the nature of the QCD transition in relativistic collision of heavy nuclei with deep learning," *Eur. Phys. J. C* **80** (6), 516, arXiv:1910.11530 [hep-ph].
- J. Duris, *et al.* (2020), "Bayesian optimization of a free-electron laser," *Phys. Rev. Lett.* **124**, 124801.
- A. Edelen, C. Mayes, D. Bowring, D. Ratner, A. Adelmann, R. Ischebeck, J. Snuverink, I. Agapov, R. Kammering, J. Edelen, I. Bazarov, G. Valentino, and J. Wenninger (2018), "Opportunities in machine learning for particle accelerators," arXiv:1811.03172 [physics.acc-ph].
- A. Edelen, N. Neveu, M. Frey, Y. Huber, C. Mayes, and A. Adelmann (2020), "Machine learning for orders of magnitude speedup in multiobjective optimization of particle accelerator systems," *Phys. Rev. Accel. Beams* **23** (4), 044601.
- C. Eklind (2021), *Eigenvector continuation and strongly interacting cold atom systems*, Ph.D. thesis <https://hdl.handle.net/20.500.12380/302455>.
- A. Ekström, and G. Hagen (2019), "Global sensitivity analysis of bulk properties of an atomic nucleus," *Phys. Rev. Lett.* **123**, 252501.
- A. Ekström (2020), "Analyzing the nuclear interaction: Challenges and new ideas," *Front. Phys.* **8**, 29.
- A. Ekström, C. Forssén, C. Dimitrakakis, D. Dubhashi, H. T. Johansson, A. S. Muhammad, H. Salomonsson, and A. Schliep (2019), "Bayesian optimization in ab initio nuclear physics," *J. Phys. G* **46** (9), 095101.
- C. Emma, A. Edelen, M. Hogan, B. O'Shea, G. White, and V. Yakimenko (2018), "Machine learning-based longitudinal phase space prediction of particle accelerators," *Phys. Rev. Accel. Beams* **21** (11), 112802.
- G. P. Engel, and S. Schaefer (2011), "Testing trivializing maps in the Hybrid Monte Carlo algorithm," *Comput. Phys. Commun.* **182**, 2107–2114.
- J. Erdmann (2020), "A tagger for strange jets based on tracking information using long short-term memory," *J. Instrum.* **15** (01), P01021.
- R. Essick, I. Tews, P. Landry, and A. Schwenk (2021), "Astrophysical constraints on the symmetry energy and the neutron skin of ^{208}Pb with minimal modeling assumptions," arXiv:2102.10074 [nucl-th].
- J. J. Ethier, N. Sato, and W. Melnitchouk (2017), "First simultaneous extraction of spin-dependent parton distributions and fragmentation functions from a global QCD analysis," *Phys. Rev. Lett.* **119** (13), 132001.
- C. Fanelli (2020), "Machine learning for imaging Cherenkov detectors," *J. Instrum.* **15** (02), C02012.
- C. Fanelli, and J. Pomponi (2020), "DeepRICH: Learning Deeply Cherenkov Detectors," *Mach. Learn.: Sci. Technol.* **1**, 015010.
- M. Favoni, A. Ipp, D. I. Müller, and D. Schuh (2020), "Lattice gauge equivariant convolutional neural networks," arXiv:2012.12901 [hep-lat].
- S. Foreman, X.-Y. Jin, and J. C. Osborn (2021), "Deep learning Hamiltonian Monte Carlo," in *9th International Conference on Learning Representations*, arXiv:2105.03418 [hep-lat].
- J. A. Formaggio, A. L. C. de Gouvêa, and R. G. H. Robertson (2021), "Direct measurements of neutrino mass," *Phys. Rept.* **914**, 1–54.
- J. M. R. Fox, C. W. Johnson, and R. N. Perez (2020), "Uncertainty quantification of an empirical shell-model interaction using principal component analysis," *Phys. Rev. C* **101**, 054308.
- S. Fraker (2018), "Deep learning for liquid-scintillator-based double-beta decay searches," 10.5281/zenodo.1300914.
- D. Frame, R. He, I. Ipsen, D. Lee, D. Lee, and E. Rrapaj (2018), "Eigenvector continuation with subspace learning," *Phys. Rev. Lett.* **121**, 032501.
- Y. Fujimoto, K. Fukushima, and K. Murase (2021), "Extensive Studies of the Neutron Star Equation of State from the Deep Learning Inference with the Observational Data Augmentation," *JHEP* **03**, 273.
- A. Fuller, Z. Fan, C. Day, and C. Barlow (2020), "Digital twin: Enabling technologies, challenges and open research," *IEEE Access* **8**, 108952–108971.
- R. Furnstahl, A. Garcia, P. Millican, and X. Zhang (2020), "Efficient emulators for scattering using eigenvector continuation," *Phys. Lett. B* **809**, 135719.
- A. Gando, *et al.* (KamLAND-Zen) (2016), "Search for Majorana neutrinos near the inverted mass hierarchy region with KamLAND-Zen," *Phys. Rev. Lett.* **117** (8), 082503, [Addendum: Phys.Rev.Lett. 117, 109903 (2016)].
- Y. Gao, J. Chen, T. Robertazzi, and K. A. Brown (2019), "Reinforcement learning based schemes to manage client activities in large distributed control systems," *Phys. Rev. Accel. Beams* **22**, 014601.
- Z.-P. Gao, Y.-J. Wang, H.-L. Lü, Q.-F. Li, C.-W. Shen, and L. Liu (2021), "Machine learning the nuclear mass," *Nucl. Sci. Tech.* **32** (10), 109.
- G. Gavalian, P. Thomadakis, A. Angelopoulos, V. Ziegler, and N. Chrisochoides (2020), "Using Artificial Intelligence for Particle Track Identification in CLAS12 Detector," arXiv e-prints , arXiv:2008.12860arXiv:2008.12860 [cs.CV].
- S. Gazula, J. Clark, and H. Bohr (1992), "Learning and prediction of nuclear stability by neural networks," *Nucl. Phys. A* **540** (1), 1 – 26.
- K. Gernoth, J. Clark, J. Prater, and H. Bohr (1993), "Neural network models of nuclear systematics," *Phys. Lett. B* **300** (1), 1 – 7.
- P. G. Giuliani, and J. Piekarewicz (2021), "From noise to information: The transfer function formalism for uncertainty quantification in reconstructing the nuclear density," *Phys. Rev. C* **104**, 024301.
- R. Gladen, V. Chirayath, A. Fairchild, M. Manry, A. Koymen, and A. Weiss (2020), "Efficient machine learning approach for optimizing the timing resolution of a high purity germanium detector," *Nucl. Instrum. Methods Phys. Res. A* **981**, 164505.
- V. V. Gligorov, and M. Williams (2013), "Efficient, reliable and fast high-level triggering using a bonsai boosted decision tree," *Journal of Instrumentation* **8** (02), P02013.
- A. Gnech, C. Adams, N. Brawand, G. Carleo, A. Lovato, and N. Rocco (2021), "Nuclei with up to $A = 6$ nucleons with artificial neural network wave functions," arXiv:2108.06836 [nucl-th].
- J. J. Gomez-Cadenas, *et al.* (NEXT) (2014), "Present status and future perspectives of the NEXT experiment," *Adv. High Energy Phys.* **2014**, 907067.
- I. Goodfellow, Y. Bengio, and A. Courville (2016), *Deep Learning* (The MIT Press, Cambridge, Massachusetts).
- S. Goriely, and R. Capote (2014), "Uncertainties of mass extrapolations in Hartree-Fock-Bogoliubov mass models," *Phys. Rev. C* **89**, 054318.

- M. Grieves, and J. Vickers (2017), “Digital twin: Mitigating unpredictable, undesirable emergent behavior in complex systems,” in *Transdisciplinary Perspectives on Complex Systems: New Findings and Approaches*, edited by F.-J. Kahlen, S. Flumerfelt, and A. Alves (Springer International Publishing, Cham) pp. 85–113.
- J. Gruszko (2018), “NuDot: double-beta decay with direction reconstruction in liquid scintillator,” [10.5281/zenodo.1300693](https://arxiv.org/abs/1803.0693).
- D. Guest, K. Cranmer, and D. Whiteson (2018), “Deep Learning and its Application to LHC Physics,” *Ann.Rev.Nucl.Part.Sci.* **68**, 161–181.
- H. Güven, K. Bozkurt, E. Khan, and J. Margueron (2020), “Multimessenger and multiphysics Bayesian inference for the GW170817 binary neutron star merger,” *Phys. Rev. C* **102**, 015805.
- D. C. Hackett, C.-C. Hsieh, M. S. Albergo, D. Boyda, J.-W. Chen, K.-F. Chen, K. Cranmer, G. Kanwar, and P. E. Shanahan (2021), “Flow-based sampling for multimodal distributions in lattice field theory,” [arXiv:2107.00734 \[hep-lat\]](https://arxiv.org/abs/2107.00734).
- A. Hamaker, E. Leistenschneider, R. Jain, G. Bollen, S. A. Giuliani, K. Lund, W. Nazarewicz, L. Neufcourt, C. R. Nicoloff, D. Puentes, R. Ringle, C. S. Sumithrarachchi, and I. T. Yandow (2021), “Precision mass measurement of lightweight self-conjugate nucleus ^{80}Zr ,” *Nat. Phys.* **10**, 1038–s41567-021-01395-w.
- M.-Z. Han, J.-L. Jiang, S.-P. Tang, and Y.-Z. Fan (2021), “Bayesian nonparametric inference of the neutron star equation of state via a neural network,” *ApJ* **919** (1), 11.
- A. Hanuka, C. Emma, T. Maxwell, A. S. Fisher, B. Jacobson, M. J. Hogan, and Z. Huang (2021), “Accurate and confident prediction of electron beam longitudinal properties using spectral virtual diagnostics,” *Sci. Rep.* **11** (1), 1–10.
- Y. Hao, Y. Li, M. Balcewicz, L. Neufcourt, and W. Cheng (2019), “Reconstruction of storage ring’s linear optics with Bayesian inference,” [arXiv preprint arXiv:1902.11157](https://arxiv.org/abs/1902.11157).
- J. Hardin, and M. Williams (2016), “FastDIRC: a fast Monte Carlo and reconstruction algorithm for DIRC detectors,” *J. Instrum.* **11** (10), P10007.
- L. A. Harland-Lang, A. D. Martin, P. Motylinski, and R. S. Thorne (2015), “Parton distributions in the LHC era: MMHT 2014 PDFs,” *Eur. Phys. J. C* **75** (5), 204.
- K. Hashimoto (2019), “AdS/CFT correspondence as a deep Boltzmann machine,” *Phys. Rev. D* **99** (10), 106017.
- K. Hashimoto, H.-Y. Hu, and Y.-Z. You (2021), “Neural ordinary differential equation and holographic quantum chromodynamics,” *Mach. Learn. Sci. Tech.* **2** (3), 035011, [arXiv:2006.00712 \[hep-th\]](https://arxiv.org/abs/2006.00712).
- K. Hashimoto, S. Sugishita, A. Tanaka, and A. Tomiya (2018a), “Deep Learning and Holographic QCD,” *Phys. Rev. D* **98** (10), 106014, [arXiv:1809.10536 \[hep-th\]](https://arxiv.org/abs/1809.10536).
- K. Hashimoto, S. Sugishita, A. Tanaka, and A. Tomiya (2018b), “Deep learning and the AdS/CFT correspondence,” *Phys. Rev. D* **98** (4), 046019, [arXiv:1802.08313 \[hep-th\]](https://arxiv.org/abs/1802.08313).
- T. Hastie, R. Tibshirani, and J. Friedman (2009), *The Elements of Statistical Learning: Data Mining, Inference and Prediction* (Springer Verlag, Berlin).
- G. Hautier, C. C. Fischer, A. Jain, T. Mueller, and G. Ceder (2010), “Finding nature’s missing ternary oxide compounds using machine learning and density functional theory,” *Chem. Mater.* **22** (12), 3762–3767.
- S. Hayashida (2019), “Application of the RNN in the fundamental physics with KamLAND experiment,” in *8th Edition of International Conference on Big Data & Data Science, Barcelona, Spain, March 04-05, 2019*.
- J. He, W.-B. He, Y.-G. Ma, and S. Zhang (2021), “Machine-learning-based identification for initial clustering structure in relativistic heavy-ion collisions,” [arXiv:2109.06277 \[hep-ph\]](https://arxiv.org/abs/2109.06277).
- Y. He, L.-G. Pang, and X.-N. Wang (2019), “Bayesian extraction of jet energy loss distributions in heavy-ion collisions,” *Phys. Rev. Lett.* **122** (25), 252302, [1808.05310](https://arxiv.org/abs/1808.05310).
- F. Heim, P. Scholz, J. Mayer, M. Müller, and A. Zilges (2020), “Constraining nuclear properties in ^{94}Mo via a $^{93}\text{Nb}(p,\gamma)^{94}\text{Mo}$ total cross section measurement,” *Phys. Rev. C* **101**, 035807.
- D. Higdon, J. D. McDonnell, N. Schunck, J. Sarich, and S. M. Wild (2015), “A Bayesian approach for parameter estimation and prediction using a computationally intensive model,” *J. Phys. G* **42** (3), 034009.
- S. Hirlaender, and N. Bruchon (2020), “Model-free and Bayesian ensembling model-based deep reinforcement learning for particle accelerator control demonstrated on the FERMI FEL,” [arXiv preprint arXiv:2012.09737](https://arxiv.org/abs/2012.09737).
- M. Hjorth-Jensen, M. P. Lombardo, and E. van Kolck, Ubirajara (2017), *An Advanced Course in Computational Nuclear Physics; Bridging the Scales from Quarks to Neutron Stars* (Springer Verlag, Berlin).
- P. Holl, L. Hauertmann, B. Majorovits, O. Schulz, M. Schuster, and A. J. Zsigmond (2019), “Deep learning based pulse shape discrimination for germanium detectors,” *Eur. Phys. J. C* **79** (6), 450.
- J. Horak, J. M. Pawłowski, J. Rodríguez-Quintero, J. Turnwald, J. M. Urban, N. Wink, and S. Zafeiropoulos (2021), “Reconstructing QCD Spectral Functions with Gaussian Processes,” [arXiv:2107.13464 \[hep-ph\]](https://arxiv.org/abs/2107.13464).
- T.-J. Hou, et al. (2021), “New CTEQ global analysis of quantum chromodynamics with high-precision data from the LHC,” *Phys. Rev. D* **103** (1), 014013.
- M. E. Houle, H.-P. Kriegel, P. Kröger, E. Schubert, and A. Zimek (2010), “Can shared-neighbor distances defeat the curse of dimensionality?” in *Int. Conf. Sci. Stat. Database Manag.* (Springer) pp. 482–500.
- B. Hu, W. Jiang, T. Miyagi, Z. Sun, A. Ekström, C. Forssén, G. Hagen, J. D. Holt, T. Papenbrock, S. R. Stroberg, and I. Vernon (2021), “Ab initio predictions link the neutron skin of ^{208}Pb to nuclear forces,” [arXiv:2112.01125 \[nucl-th\]](https://arxiv.org/abs/2112.01125).
- Y.-G. Huang, L.-G. Pang, X. Luo, and X.-N. Wang (2021), “Probing criticality with deep learning in relativistic heavy-ion collisions,” [arXiv:2107.11828 \[nucl-th\]](https://arxiv.org/abs/2107.11828).
- D. Huber, O. V. Marchukov, H.-W. Hammer, and A. G. Volosniev (2021), “Morphology of three-body quantum states from machine learning,” *New J. Phys.* **23** (6), 065009.
- N. Ismail, and A. Gezerlis (2021), “Machine-learning approach to finite-size effects in systems with strongly interacting fermions,” *Phys. Rev. C* **104**, 055802.
- A. Jany, et al. (2021), “Fabrication, characterization and analysis of a prototype high purity germanium detector for ^{76}Ge -based neutrinoless double beta decay experiments,” *Eur. Phys. J. C* **81** (1), 38.
- C. Jiang, B. Szymanski, J. Lian, S. Havlin, and J. Gao (2021), “Nuclear reaction network unveils novel reaction patterns based on stellar energies,” *New J. Phys.* **23**, 083035.
- W. G. Jiang, G. Hagen, and T. Papenbrock (2019), “Extrapolation of nuclear structure observables with artificial

- neural networks,” *Phys. Rev. C* **100**, 054326.
- J. S. John, M. Schram, C. Herwig, D. Kafkes, J. Mitrevski, W. A. Pellico, G. N. Perdue, A. Quintero-Parra, B. A. Schupbach, K. Seiya, N. Tran, J. M. Duarte, Y. Huang, and R. Keller (2021), “Real-time artificial intelligence for accelerator control: A study at the fermilab booster,” [arXiv:2011.07371 \[physics.acc-ph\]](https://arxiv.org/abs/2011.07371).
- D. R. Jones, M. Schonlau, and W. J. Welch (1998), “Efficient global optimization of expensive black-box functions,” *J. Global Optim.* **13** (4), 455–492.
- D. Kafkes, and M. Schram (2021), “Developing Robust Digital Twins and Reinforcement Learning for Accelerator Control Systems at the Fermilab Booster,” in *12th IPAC 2021*, [arXiv:2105.12847 \[physics.acc-ph\]](https://arxiv.org/abs/2105.12847).
- V. Kain, S. Hirlander, B. Goddard, F. M. Velotti, G. Z. Della Porta, N. Bruchon, and G. Valentino (2020), “Sample-efficient reinforcement learning for CERN accelerator control,” *Phys. Rev. Accel. Beams* **23** (12), 124801.
- M. Kamuda, J. Stinnett, and C. J. Sullivan (2017), “Automated isotope identification algorithm using artificial neural networks,” *IEEE Trans. Nucl. Sci.* **64** (7), 1858–1864.
- M. Kamuda, and C. J. Sullivan (2018), “An automated isotope identification and quantification algorithm for isotope mixtures in low-resolution gamma-ray spectra,” *Radiat. Phys. Chem.* **155**, 10.1016/j.radphyschem.2018.06.017.
- M. Kamuda, J. Zhao, and K. Huff (2020), “A comparison of machine learning methods for automated gamma-ray spectroscopy,” *Nucl. Instr. Meth. Phys. Res. A* **954**, 161385.
- G. Kanwar, M. S. Albergo, D. Boyd, K. Cranmer, D. C. Hackett, S. Racanière, D. J. Rezende, and P. E. Shanahan (2020), “Equivariant flow-based sampling for lattice gauge theory,” *Phys. Rev. Lett.* **125** (12), 121601.
- J. Karpie, K. Orginos, A. Rothkopf, and S. Zafeiropoulos (2019), “Reconstructing parton distribution functions from Ioffe time data: from Bayesian methods to Neural Networks,” *JHEP* **04**, 057.
- B. Kapschak, and U.-G. Meißner (2021), “Neural network perturbation theory and its application to the Born series,” *Phys. Rev. Research* **3**, 023223.
- J. Keeble, and A. Rios (2020), “Machine learning the deuteron,” *Phys. Lett. B* **809**, 135743.
- V. Kejzlar, L. Neufcourt, W. Nazarewicz, and P.-G. Reinhard (2020), “Statistical aspects of nuclear mass models,” *J. Phys. G* **47**, 094001.
- M. Kekic, *et al.* (NEXT) (2021), “Demonstration of background rejection using deep convolutional neural networks in the NEXT experiment,” *J. High Energ. Phys.* **01**, 189.
- R. A. Khalek, *et al.* (2021), “Science requirements and detector concepts for the Electron-Ion Collider: EIC Yellow Report,” [arXiv:2103.05419v3 \[physics.ins-det\]](https://arxiv.org/abs/2103.05419v3).
- G. B. King, A. E. Lovell, L. Neufcourt, and F. M. Nunes (2019), “Direct comparison between Bayesian and frequentist uncertainty quantification for nuclear reactions,” *Phys. Rev. Lett.* **122** (23), 232502.
- R. Koenker, and G. Bassett (1978), “Regression quantiles,” *Econometrica* **46**, 211–244.
- A. Koesdiady, S. Bedawi, C. Ou, and F. Karray (2018), “Non-stationary traffic flow prediction using deep learning,” in *Proc. 88th Vehicular Tech. Conf.* (IEEE) pp. 1–5.
- P. T. Komiske, E. M. Metodiev, B. Nachman, and M. D. Schwartz (2017a), “Pileup mitigation with machine learning,” [arXiv:1707.08600 \[hep-ex\]](https://arxiv.org/abs/1707.08600).
- P. T. Komiske, E. M. Metodiev, and M. D. Schwartz (2017b), “Deep learning in color: towards automated quark/gluon jet discrimination,” *J. High Energy Phys.* **2017** (1), 1–23.
- L. Kramárik (STAR) (2020), “Reconstruction of D^0 meson in d+Au collisions at $\sqrt{s_{NN}} = 200$ GeV by the STAR experiment,” *Phys. Scripta* **95** (7), 074010.
- M. Kranjčević, B. Riemann, A. Adelmann, and A. Streun (2021), “Multiobjective optimization of the dynamic aperture using surrogate models based on artificial neural networks,” *Phys. Rev. Accel. Beams* **24** (1), 014601.
- K. Kravvaris, K. R. Quinlan, S. Quaglioni, K. A. Wendt, and P. Navrátil (2020), “Quantifying uncertainties in neutron- α scattering with chiral nucleon-nucleon and three-nucleon forces,” *Phys. Rev. C* **102**, 024616.
- M. P. Kuchera, R. Ramanujan, J. Z. Taylor, R. R. Strauss, D. Bazin, J. Bradt, and R. Chen (2019), “Machine learning methods for track classification in the AT-TPC,” *Nucl. Instrum. Meth. Phys. Res. A* **940**, 156–167.
- N. Kunert, P. T. H. Pang, I. Tews, M. W. Coughlin, and T. Dietrich (2021), “Quantifying modelling uncertainties when combining multiple gravitational-wave detections from binary neutron star sources,” [arXiv:2110.11835 \[astro-ph.HE\]](https://arxiv.org/abs/2110.11835).
- R. Kurle, B. Cseke, A. Klushyn, P. van der Smagt, and S. Günemann (2019), “Continual learning with bayesian neural networks for non-stationary data,” in *Proc. Int. Conf. Learning Representations*.
- M. O. Kuttan, J. Steinheimer, K. Zhou, A. Redelbach, and H. Stoecker (2021), “Deep Learning Based Impact Parameter Determination for the CBM Experiment,” *Particles* **4** (1), 47–52.
- S. König, A. Ekström, K. Hebeler, D. Lee, and A. Schwenk (2020), “Eigenvector continuation as an efficient and accurate emulator for uncertainty quantification,” *Phys. Lett. B* **810**, 135814.
- R. Lasseri, D. Regnier, J. Ebran, and A. Penon (2020), “Taming nuclear complexity with a committee of multilayer neural networks,” *Phys. Rev. Lett.* **124**, 162502.
- S. Lawrence, and Y. Yamauchi (2021), “Normalizing Flows and the Real-Time Sign Problem,” *Phys. Rev. D* **103** (11), 114509, [arXiv:2101.05755 \[hep-lat\]](https://arxiv.org/abs/2101.05755).
- D. Levy, M. D. Hoffman, and J. Sohl-Dickstein (2018), “Generalizing Hamiltonian Monte Carlo with neural networks,” in *International Conference on Learning Representations*.
- A. Li, A. Elagin, S. Fraker, C. Grant, and L. Winslow (2019a), “Suppression of cosmic muon spallation backgrounds in liquid scintillator detectors Using convolutional neural networks,” *Nucl. Instrum. Meth. A* **947**, 162604.
- F. Li, Y. Wang, Z. Gao, P. Li, H. Lv, Q. Li, C. Y. Tsang, and M. B. Tsang (2021a), “Application of machine learning in the determination of impact parameter in the $^{132}\text{Sn} + ^{124}\text{Sn}$ system,” [arXiv:2105.08912 \[nucl-th\]](https://arxiv.org/abs/2105.08912).
- F. Li, Y. Wang, H. Lü, P. Li, Q. Li, and F. Liu (2020a), “Application of artificial intelligence in the determination of impact parameter in heavy-ion collisions at intermediate energies,” *J. Phys. G* **47** (11), 115104.
- S. Li, M. Zacharias, J. Snuverink, J. Coello de Portugal, F. Perez-Cruz, D. Reggiani, and A. Adelmann (2021b), “A novel approach for classification and forecasting of time series in particle accelerators,” *Information* **12** (3), 10.3390/info12030121.
- S.-H. Li, C.-X. Dong, L. Zhang, and L. Wang (2020b), “Neural canonical transformation with symplectic flows,” *Phys. Rev. X* **10**, 021020.
- T. Li, S. Wang, Y. Chen, K. Han, H. Lin, K. Ni, W. Wang, Y. Xu, and A. Zou (2021c), “Signal identification with

- Kalman filter towards background-free neutrinoless double beta decay searches in gaseous detectors," *J. High Energ. Phys.* **6**, 106.
- Y. Li, W. Cheng, L. H. Yu, and R. Rainer (2018a), "Genetic algorithm enhanced by machine learning in dynamic aperture optimization," *Phys. Rev. Accel. Beams* **21** (5), 054601.
- Y. Li, W. Cheng, L. H. Yu, and R. Rainer (2018b), "Genetic algorithm enhanced by machine learning in dynamic aperture optimization," *Phys. Rev. Accel. Beams* **21**, 054601.
- Y. Li, R. Rainer, and W. Cheng (2019b), "Bayesian approach for linear optics correction," *Phys. Rev. Accel. Beams* **22** (1), 012804.
- J. Liepe, S. Filippi, M. Komorowski, and M. P. H. Stumpf (2013), "Maximizing the information content of experiments in systems biology," *PLOS Comput. Biol.* **9** (1), 1–13.
- T. Likhomanenko, P. Ilten, E. Khairullin, A. Rogozhnikov, A. Ustyuzhanin, and M. Williams (2015), "Lhcb topological trigger reoptimization," in *Journal of Physics: Conference Series*, Vol. 664 (IOP Publishing) p. 082025.
- Y. Lim, and J. W. Holt (2019), "Bayesian modeling of the nuclear equation of state for neutron star tidal deformabilities and GW170817," *Eur. Phys. J. A* **55** (11), 209.
- H.-W. Lin, W. Melnitchouk, A. Prokudin, N. Sato, and H. Shows (2018), "First Monte Carlo Global Analysis of Nucleon Transversity with Lattice QCD Constraints," *Phys. Rev. Lett.* **120** (15), 152502.
- H. Liu, D. Han, Y. Ma, and L. Zhu (2020), "Network structure of thermonuclear reactions in nuclear landscape," *Sci. China Phys. Mech. & Astron.* **63** (11), 112062.
- Y. Liu, C. Su, J. Liu, P. Danielewicz, C. Xu, and Z. Ren (2021), "Improved naive Bayesian probability classifier in predictions of nuclear mass," *Phys. Rev. C* **104**, 014315.
- A. Lovell, A. Mohan, P. Talou, and M. Chertkov (2019), "Constraining fission yields using machine learning," *Eur. Phys. J. Web Conf.* **211**, 04006.
- A. Lovell, F. M. Nunes, M. Catacora-Rios, and G. King (2021), "Recent advances in the quantification of uncertainties in reaction theory," *J. Phys. G* **48**, 014001.
- A. E. Lovell, A. T. Mohan, and P. Talou (2020), "Quantifying uncertainties on fission fragment mass yields with mixture density networks," *J. Phys. G* **47** (11), 114001.
- A. E. Lovell, and F. M. Nunes (2018), "Constraining transfer cross sections using Bayes' theorem," *Phys. Rev. C* **97** (6), 064612.
- S. Lundberg, and S. Lee (2017), "A unified approach to interpreting model predictions," in *Proceedings of the 31st International Conference on Neural Information Processing Systems*, NIPS'17 (Curran Associates Inc., Red Hook, NY, USA) p. 4768–4777.
- D. Luo, G. Carleo, B. K. Clark, and J. Stokes (2020), "Gauge equivariant neural networks for quantum lattice gauge theories," [arXiv:2012.05232 \[cond-mat.str-el\]](https://arxiv.org/abs/2012.05232).
- D. Luo, Z. Chen, K. Hu, Z. Zhao, V. M. Hur, and B. K. Clark (2021), "Gauge Invariant Autoregressive Neural Networks for Quantum Lattice Models," [arXiv:2101.07243 \[cond-mat.str-el\]](https://arxiv.org/abs/2101.07243).
- M. Lüscher (2010), "Trivializing maps, the Wilson flow and the HMC algorithm," *Commun. Math. Phys.* **293**, 899–919.
- M. Lüscher (2015), "Instantaneous stochastic perturbation theory," *JHEP* **04**, 142.
- C. Ma, D. Peng, H. Wei, Z. Niu, Y. Wang, and R. Wada (2020a), "Isotopic cross-sections in proton induced spallation reactions based on the Bayesian neural network method," *Chin. Phys. C* **44** (1), 014104.
- Y. Ma, C. Su, J. Liu, Z. Ren, C. Xu, and Y. Gao (2020b), "Predictions of nuclear charge radii and physical interpretations based on the naive Bayesian probability classifier," *Phys. Rev. C* **101**, 014304.
- A. Maevskiy, D. Derkach, N. Kazeev, A. Ustyuzhanin, M. Artemev, L. Anderlini, L. Collaboration, *et al.* (2020), "Fast Data-Driven Simulation of Cherenkov Detectors Using Generative Adversarial Networks," in *J. Phys. Conf. Ser.*, Vol. 1525 (IOP Publishing) p. 012097.
- A. Magilligan, and B. A. Brown (2020), "New isospin-breaking "USD" Hamiltonians for the sd shell," *Phys. Rev. C* **101**, 064312.
- D. Maksimović, M. Nieslony, and M. Wurm (2021), "CNNs for enhanced background discrimination in DSNB searches in large-scale water-Gd detectors," [arXiv:2104.13426 \[physics.ins-det\]](https://arxiv.org/abs/2104.13426).
- N. Mallick, S. Tripathy, A. N. Mishra, S. Deb, and R. Sahoo (2021), "Estimation of Impact Parameter and Transverse Spherocity in heavy-ion collisions at the LHC energies using Machine Learning," [arXiv:2103.01736 \[hep-ph\]](https://arxiv.org/abs/2103.01736).
- J. T. Margraf, and K. Reuter (2018), "Making the coupled cluster correlation energy machine learnable," *J. Phys. Chem. A* **122**, 6343.
- J. Margueron, H. Casali, and F. Gulminelli (2018a), "Equation of state for dense nucleonic matter from metamodeling. I. Foundational aspects," *Phys. Rev. C* **97**, 025805.
- J. Margueron, H. Casali, and F. Gulminelli (2018b), "Equation of state for dense nucleonic matter from metamodeling. II. Predictions for neutron star properties," *Phys. Rev. C* **97**, 025806.
- J. D. McDonnell, N. Schunck, D. Higdon, J. Sarich, S. M. Wild, and W. Nazarewicz (2015), "Uncertainty quantification for nuclear density functional theory and information content of new measurements," *Phys. Rev. Lett.* **114**, 122501.
- L. McInnes, J. Healy, and S. Astels (2017), "hdbscan: Hierarchical density based clustering," *Journal of Open Source Software* **2** (11), 205.
- M. McIntire, T. Cope, S. Ermon, D. Ratner, *et al.* (2016), "Bayesian optimization of FEL performance at LCLS," in *Proc. 7th Int. Particle Accelerator Conf.*
- M. Medhat (2012), "Artificial intelligence methods applied for quantitative analysis of natural radioactive sources," *Ann. Nucl. Energy* **45**, 73–79.
- M. Medvidovic, J. Carrasquilla, L. E. Hayward, and B. Kulchytskyy (2020), "Generative models for sampling of lattice field theories," in *34th Conference on Neural Information Processing Systems*, [arXiv:2012.01442 \[cond-mat.dis-nn\]](https://arxiv.org/abs/2012.01442).
- P. Mehta, M. Bukov, C. Wang, A. G. Day, C. Richardson, C. K. Fisher, and D. J. Schwab (2019), "A high-bias, low-variance introduction to machine learning for physicists," *Phys. Rep.* **810**, 1 – 124.
- J. Melendez, C. Drischler, A. Garcia, R. Furnstahl, and X. Zhang (2021a), "Fast & accurate emulation of two-body scattering observables without wave functions," *Phys. Lett. B* **821**, 136608.
- J. A. Melendez, R. J. Furnstahl, H. W. Grießhammer, J. A. McGovern, D. R. Phillips, and M. T. Pratola (2021b), "Designing optimal experiments: An application to proton Compton scattering," *Eur. Phys. J. A* **57** (3), 81.
- J. A. Melendez, R. J. Furnstahl, D. R. Phillips, M. T. Pra-

- tola, and S. Wesolowski (2019), “Quantifying correlated truncation errors in effective field theory,” *Phys. Rev. C* **100**, 044001.
- J. A. Melendez, S. Wesolowski, and R. J. Furnstahl (2017), “Bayesian truncation errors in chiral effective field theory: Nucleon-nucleon observables,” *Phys. Rev. C* **96**, 024003.
- I. Michaud, N. Kleedtke, J. Hutchinson, T. Smith, R. Little, T. Grove, and M. Rising (2019), “Designing critical experiments using Gaussian process optimization,” *Trans. Am. Nucl. Soc.* **121**, 1035–1038.
- M. C. Miller, C. Chirenti, and F. K. Lamb (2020), “Constraining the equation of state of high-density cold matter using nuclear and astronomical measurements,” *ApJ* **888** (1), 12.
- E. Moffat, W. Melnitchouk, T. Rogers, and N. Sato (2021), “Simultaneous Monte Carlo analysis of parton densities and fragmentation functions,” [arXiv:2101.04664 \[hep-ph\]](https://arxiv.org/abs/2101.04664).
- O. M. Molchanov, K. D. Launey, A. Mercenne, G. H. Sargsyan, T. Dytrych, and J. P. Draayer (2021), “Machine learning approach to pattern recognition in nuclear dynamics from the ab initio symmetry-adapted no-core shell model,” [arXiv:2107.01498 \[nucl-th\]](https://arxiv.org/abs/2107.01498).
- B. Montreal, and J. A. Formaggio (2009), “Relativistic cyclotron radiation detection of tritium decay electrons as a new technique for measuring the neutrino mass,” *Phys. Rev. D* **80**, 051301.
- J. R. Moreno, G. Carleo, and A. Georges (2020), “Deep learning the Hohenberg-Kohn maps of density functional theory,” *Phys. Rev. Lett.* **125**, 076402.
- P. Morfouace, *et al.* (2019), “Constraining the symmetry energy with heavy-ion collisions and Bayesian analyses,” *Phys. Lett. B* **799**, 135045.
- K. P. Murphy (2012), *Machine Learning: A Probabilistic Perspective* (The MIT Press, Cambridge, Massachusetts).
- S. Myren, and E. Lawrence (2021), “A comparison of Gaussian processes and neural networks for computer model emulation and calibration,” *Stat. Anal. Data Min.* **n/a**, 11507.
- R. Nagai, R. Akashi, and O. Sugino (2020), “Completing density functional theory by machine learning hidden messages from molecules,” *Npj Comput. Mater.* **6** (1), 43.
- Y. Nakai, D. Shih, and S. Thomas (2020), “Strange jet tagging,” [arXiv:2003.09517v1 \[hep-ph\]](https://arxiv.org/abs/2003.09517v1).
- A. Nandi, C. Qu, P. L. Houston, R. Conte, and J. M. Bowman (2021), “ Δ -machine learning for potential energy surfaces: A PIP approach to bring a DFT-based PES to CCSD(T) level of theory,” *J. Chem. Phys.* **154** (5), 051102.
- Nätilä, J., Miller, M. C., Steiner, A. W., Kajava, J. J. E., Suleimanov, V. F., and Poutanen, J. (2017), “Neutron star mass and radius measurements from atmospheric model fits to X-ray burst cooling tail spectra,” *A&A* **608**, A31.
- R. Navarro Pérez, J. E. Amaro, E. Ruiz Arriola, P. Maris, and J. P. Vary (2015), “Statistical error propagation in ab initio no-core full configuration calculations of light nuclei,” *Phys. Rev. C* **92**, 064003.
- R. Navarro Pérez, N. Schunck, A. Dyhdalo, R. J. Furnstahl, and S. K. Bogner (2018), “Microscopically based energy density functionals for nuclei using the density matrix expansion. II. Full optimization and validation,” *Phys. Rev. C* **97**, 054304.
- G. A. Negoita, J. P. Vary, G. R. Luecke, P. Maris, A. M. Shirokov, I. J. Shin, Y. Kim, E. G. Ng, C. Yang, M. Lockner, and G. M. Prabhu (2019), “Deep learning: Extrapolation tool for ab initio nuclear theory,” *Phys. Rev. C* **99**, 054308.
- D. Neudecker, O. Cabellos, A. R. Clark, M. J. Grosskopf, W. Haeck, M. W. Herman, J. Hutchinson, T. Kawano, A. E. Lovell, I. Stetcu, P. Talou, and S. Vander Wiel (2021), “Informing nuclear physics via machine learning methods with differential and integral experiments,” *Phys. Rev. C* **104**, 034611.
- D. Neudecker, M. Grosskopf, M. Herman, W. Haeck, P. Grechanuk, S. Vander Wiel, M. Rising, A. Kahler, N. Sly, and P. Talou (2020), “Enhancing nuclear data validation analysis by using machine learning,” *Nucl. Data Sheets* **167**, 36–60.
- L. Neufcourt, Y. Cao, S. Giuliani, W. Nazarewicz, E. Olsen, and O. B. Tarasov (2020a), “Beyond the proton drip line: Bayesian analysis of proton-emitting nuclei,” *Phys. Rev. C* **101**, 014319.
- L. Neufcourt, Y. Cao, S. A. Giuliani, W. Nazarewicz, E. Olsen, and O. B. Tarasov (2020b), “Quantified limits of the nuclear landscape,” *Phys. Rev. C* **101**, 044307.
- L. Neufcourt, Y. Cao, W. Nazarewicz, E. Olsen, and F. Viens (2019), “Neutron drip line in the Ca region from Bayesian model averaging,” *Phys. Rev. Lett.* **122**, 062502.
- L. Neufcourt, Y. Cao, W. Nazarewicz, and F. Viens (2018), “Bayesian approach to model-based extrapolation of nuclear observables,” *Phys. Rev. C* **98**, 034318.
- N. Neveu, L. Spentzouris, A. Adelmann, Y. Ineichen, A. Kolano, C. Metzger-Kraus, C. Bekas, A. Curioni, and P. Arbenz (2019), “Parallel general purpose multiobjective optimization framework with application to electron beam dynamics,” *Phys. Rev. Accel. Beams* **22**, 054602.
- W. G. Newton, and G. Crocombe (2021), “Nuclear symmetry energy from neutron skins and pure neutron matter in a Bayesian framework,” *Phys. Rev. C* **103**, 064323.
- K. A. Nicoli, C. J. Anders, L. Funcke, T. Hartung, K. Jansen, P. Kessel, S. Nakajima, and P. Stornati (2021), “Estimation of Thermodynamic Observables in Lattice Field Theories with Deep Generative Models,” *Phys. Rev. Lett.* **126** (3), 032001.
- Z. Niu, and H. Liang (2018), “Nuclear mass predictions based on Bayesian neural network approach with pairing and shell effects,” *Phys. Lett. B* **778**, 48 – 53.
- Z. M. Niu, J. Y. Fang, and Y. F. Niu (2019a), “Comparative study of radial basis function and Bayesian neural network approaches in nuclear mass predictions,” *Phys. Rev. C* **100**, 054311.
- Z. M. Niu, H. Z. Liang, B. H. Sun, W. H. Long, and Y. F. Niu (2019b), “Predictions of nuclear β -decay half-lives with machine learning and their impact on r -process nucleosynthesis,” *Phys. Rev. C* **99**, 064307.
- D. R. Nygren, B. J. P. Jones, N. López-March, Y. Mei, F. Psihas, and R. J. (2018), “Neutrinoless double beta decay with 82sef6and direct ion imaging,” *JINST* **13** (03), P03015–P03015.
- D. Odell, C. Brune, and D. Phillips (2021), “How Bayesian methods can improve R -matrix analyses of data: the example of the dt Reaction,” [arXiv:2105.06541 \[nucl-th\]](https://arxiv.org/abs/2105.06541).
- A. Ohnishi, Y. Mori, and K. Kashiwa (2019), “Path Optimization for the Sign Problem in Field Theories Using Neural Network,” *JPS Conf. Proc.* **26**, 024011.
- M. Omana Kuttan, J. Steinheimer, K. Zhou, A. Redelbach, and H. Stoecker (2020), “A fast centrality-meter for heavy-ion collisions at the CBM experiment,” *Phys. Lett. B* **811**, 135872.
- F. H. O’Shea, N. Bruchon, and G. Gaio (2020), “Policy gradient methods for free-electron laser and terahertz source optimization and stabilization at the FERMI free-electron

- laser at Elettra,” *Phys. Rev. Accel. Beams* **23** (12), 122802.
- B. S. Page, X. Chu, and E. C. Aschenauer (2020), “Experimental aspects of jet physics at a future eic,” *Phys. Rev. D* **101** (7), 072003.
- L.-G. Pang, K. Zhou, N. Su, H. Petersen, H. Stöcker, and X.-N. Wang (2018), “An equation-of-state-meter of quantum chromodynamics transition from deep learning,” *Nature Commun.* **9** (1), 210.
- L.-G. Pang, K. Zhou, and X.-N. Wang (2019), “Interpretable deep learning for nuclear deformation in heavy ion collisions,” [arXiv:1906.06429 \[nucl-th\]](https://arxiv.org/abs/1906.06429).
- J.-F. Paquet, *et al.* (JETSCAPE) (2021), “Revisiting Bayesian constraints on the transport coefficients of QCD,” *Nucl. Phys. A* **1005**, 121749.
- A. Pastore, and M. Carnini (2021), “Extrapolating from neural network models: a cautionary tale,” *J. Phys. G* **48**, 084001.
- A. Pastore, D. Neill, H. Powell, K. Medler, and C. Barton (2020), “Impact of statistical uncertainties on the composition of the outer crust of a neutron star,” *Phys. Rev. C* **101**, 035804.
- J. M. Pawłowski, and J. M. Urban (2020), “Reducing Auto-correlation Times in Lattice Simulations with Generative Adversarial Networks,” *Mach. Learn. Sci. Tech.* **1**, 045011, [arXiv:1811.03533 \[hep-lat\]](https://arxiv.org/abs/1811.03533).
- G. Pederiva, and A. Shindler (2020), “Machine Learning for Hadron Correlators from lattice QCD,” Work in progress.
- D. R. Phillips, R. Furnstahl, U. Heinz, T. Maiti, W. Nazarewicz, F. Nunes, M. Plumlee, S. Pratt, M. Pratola, F. Viens, and S. M. Wild (2021), “Get on the BAND wagon: A Bayesian framework for quantifying model uncertainties in nuclear dynamics,” *J. Phys. G* **48**, 072001.
- S. Pratt, E. Sangaline, P. Sorensen, and H. Wang (2015), “Constraining the Eq. of State of Super-Hadronic Matter from Heavy-Ion Collisions,” *Phys. Rev. Lett.* **114**, 202301.
- B. Pritychenko, *et al.* (2011), “The nuclear science references (nsr) database and web retrieval system,” *Nucl. Inst. Meth. Phys. Res. A* **640**, 213.
- J. Pumplin, D. R. Stump, J. Huston, H. L. Lai, P. M. Nadolsky, and W. K. Tung (2002), “New generation of parton distributions with uncertainties from global QCD analysis,” *JHEP* **07**, 012.
- Z. Qian, *et al.* (2021), “Vertex and energy reconstruction in JUNO with machine learning methods,” *Nucl. Instrum. Meth. A* **1010**, 165527.
- C. Y. Qiao, J. C. Pei, Z. A. Wang, Y. Qiang, Y. J. Chen, N. C. Shu, and Z. G. Ge (2021), “Bayesian evaluation of charge yields of fission fragments of ^{239}U ,” *Phys. Rev. C* **103**, 034621.
- H. Qiao, C. Lu, X. Chen, K. Han, X. Ji, and S. Wang (2018), “Signal-background discrimination with convolutional neural networks in the PandaX-III experiment using MC simulation,” *Sci. China Phys. Mech. Astron.* **61** (10), 101007.
- G. Raaijmakers, S. K. Greif, T. E. Riley, T. Hinderer, K. Hebeler, A. Schwenk, A. L. Watts, S. Nissanke, S. Guillot, J. M. Lattimer, and R. M. Ludlam (2020), “Constraining the dense matter equation of state with joint analysis of NICER and LIGO/Virgo measurements,” *Astrophys. J. Lett.* **893**, L21.
- M. I. Radaideh, and T. Kozlowski (2020), “Analyzing nuclear reactor simulation data and uncertainty with the group method of data handling,” *Nuclear Engineering and Technology* **52** (2), 287–295.
- K. Raghavan, P. Balaprakash, A. Lovato, N. Rocco, and S. M. Wild (2021), “Machine-learning-based inversion of nuclear responses,” *Phys. Rev. C* **103**, 035502.
- J. Renner, *et al.* (2017), “Background rejection in NEXT using deep neural networks,” *J. Instrum.* **12** (01), T01004–T01004.
- M. Rescic, R. Seviour, and W. Blokland (2020), “Predicting particle accelerator failures using binary classifiers,” *Nucl. Instrum. Methods Phys. Res. A* **955**, 10.1016/j.nima.2019.163240.
- U. Rodríguez, C. Z. Vargas, M. Gonçalves, S. B. Duarte, and F. Guzmán (2019a), “Alpha half-lives calculation of superheavy nuclei with $Q\alpha$ -value predictions based on the Bayesian neural network approach,” *J. Phys. G* **46** (11), 115109.
- U. B. Rodríguez, C. Z. Vargas, M. Gonçalves, S. B. Duarte, and F. Guzmán (2019b), “Bayesian neural network improvements to nuclear mass formulae and predictions in the superheavy elements region,” *EPL* **127** (4), 42001.
- C. Romano, *et al.* (2020), “Proceedings of the workshop for applied nuclear data: Wanda 2020,” .
- E. Rrapaj, and A. Roggero (2021), “Exact representations of many-body interactions with restricted-Boltzmann-machine neural networks,” *Phys. Rev. E* **103**, 013302.
- D. E. Rumelhart, G. E. Hinton, and R. J. Williams (1986), “Learning representations by back-propagating errors,” *Nature* **323** (6088), 533–536.
- K. Ryczko, D. A. Strubbe, and I. Tamblyn (2019), “Deep learning and density-functional theory,” *Phys. Rev. A* **100**, 022512.
- H. Saito (2018), “Method to solve quantum few-body problems with artificial neural networks,” *J. Phys. Soc. Jpn.* **87** (7), 074002.
- A. Sarkar, and D. Lee (2021), “Self-learning Emulators and Eigenvector Continuation,” [arXiv:2107.13449 \[nucl-th\]](https://arxiv.org/abs/2107.13449).
- N. Sato, C. Andres, J. J. Ethier, and W. Melnitchouk (JAM) (2020), “Strange quark suppression from a simultaneous Monte Carlo analysis of parton distributions and fragmentation functions,” *Phys. Rev. D* **101** (7), 074020.
- G. Saxena, P. K. Sharma, and P. Saxena (2021), “Modified empirical formulas and machine learning for α -decay systematics,” *J. Phys. G* **48** (5), 055103.
- G. Scamps, S. Goriely, E. Olsen, M. Bender, and W. Ryssens (2020), “Grid Skyrme functional obtained using a committee of multilayer neural networks,” [arXiv:2011.07904 \[nucl-th\]](https://arxiv.org/abs/2011.07904).
- S. Schaefer, R. Sommer, and F. Virotta (ALPHA) (2011), “Critical slowing down and error analysis in lattice QCD simulations,” *Nucl. Phys. B* **845**, 93–119.
- A. Scheinker (2013), “Model independent beam tuning,” in *Proc. 2013 Int. Particle Accelerator Conf.*
- A. Scheinker (2021), “Adaptive machine learning for time-varying systems: low dimensional latent space tuning,” *J. Instrum.* **16** (10), <https://doi.org/10.1088/1748-0221/16/10/p10008>.
- A. Scheinker, D. Bohler, S. Tomin, R. Kammering, I. Zagorodnov, H. Schlarb, M. Scholz, B. Beutner, and W. Decking (2019), “Model-independent tuning for maximizing free electron laser pulse energy,” *Phys. Rev. Accel. Beams* **22** (8), 082802.
- A. Scheinker, F. Croppe, S. Paiagua, and D. Filippetto (2021), “An adaptive approach to machine learning for compact particle accelerators,” *Sci. Rep.* <https://doi.org/10.1038/s41598-021-98785-0>.
- A. Scheinker, A. Edelen, D. Bohler, C. Emma, and A. Lut-

- man (2018), “Demonstration of model-independent control of the longitudinal phase space of electron beams in the linac-coherent light source with femtosecond resolution,” *Phys. Rev. Lett.* **121** (4), 044801.
- A. Scheinker, C. Emma, A. L. Edelen, and S. Gessner (2020a), “Advanced control methods for particle accelerators (acm4pa) 2019 workshop report,” [arXiv:2001.05461 \[physics.acc-ph\]](https://arxiv.org/abs/2001.05461).
- A. Scheinker, and S. Gessner (2015), “Adaptive method for electron bunch profile prediction,” *Phys. Rev. Accel. Beams* **18** (10), 102801.
- A. Scheinker, S. Gessner, C. Emma, and A. L. Edelen (2020b), “Adaptive model tuning studies for non-invasive diagnostics and feedback control of plasma wakefield acceleration at FACET-II,” *Nucl. Instrum. Methods Phys. Res. A: Accel. Spectrom. Detect. Assoc. Equip.* **967**, 163902.
- A. Scheinker, S. Hirlaender, F. M. Velotti, S. Gessner, G. Z. Della Porta, V. Kain, B. Goddard, and R. Ramjiawan (2020c), “Online multi-objective particle accelerator optimization of the AWAKE electron beam line for simultaneous emittance and orbit control,” *AIP Adv.* **10** (5), 055320.
- A. Scheinker, and M. Krstić (2017), *Model-free stabilization by extremum seeking* (Springer).
- A. Scheinker, and D. Scheinker (2021), “Extremum seeking for optimal control problems with unknown time-varying systems and unknown objective functions,” *Int. J. Adapt. Control* **35** (7), 1143–1161.
- G. R. Schleider, A. C. M. Padilha, C. M. Acosta, M. Costa, and A. Fazzio (2019), “From DFT to machine learning: recent approaches to materials science—a review,” *J. Phys. Mat.* **2** (3), 032001.
- G. Schnabel, R. Capote, A. Koning, and D. Brown (2021), “Nuclear data evaluation with bayesian networks,” [arXiv:2110.10322](https://arxiv.org/abs/2110.10322).
- G. Schnabel, *et al.* (2020), “Conception and software implementation of a nuclear data evaluation pipeline,” [arXiv:2009.00521v1](https://arxiv.org/abs/2009.00521v1).
- N. Schunck, Ed. (2019), *Energy Density Functional Methods for Atomic Nuclei*, 2053–2563 (IOP Publishing, Bristol, UK).
- N. Schunck, J. O’Neal, M. Grosskopf, E. Lawrence, and S. M. Wild (2020a), “Calibration of energy density functionals with deformed nuclei,” *J. Phys. G* **47** (7), 074001.
- N. Schunck, K. R. Quinlan, and J. Bernstein (2020b), “A Bayesian analysis of nuclear deformation properties with Skyrme energy functionals,” *J. Phys. G* **47** (10), 104002.
- R. J. Shalloo, S. J. D. Dann, J. N. Gruse, C. I. D. Underwood, A. F. Antoine, C. Arran, M. Backhouse, C. D. Baird, M. D. Balcazar, N. Bourgeois, *et al.* (2020), “Automation and control of laser wakefield accelerators using Bayesian optimization,” *Nat. Commun.* **11** (1), 1–8.
- P. E. Shanahan, D. Trewartha, and W. Detmold (2018), “Machine learning action parameters in lattice quantum chromodynamics,” *Phys. Rev. D* **97** (9), 094506, [arXiv:1801.05784 \[hep-lat\]](https://arxiv.org/abs/1801.05784).
- M. Shelley, and A. Pastore (2021), “A new mass model for nuclear astrophysics: Crossing 200 keV accuracy,” *Universe* **7** (5), 131.
- Y. F. Shen, R. Pokharel, T. J. Nizolek, A. Kumar, and T. Lookman (2019), “Convolutional neural network-based method for real-time orientation indexing of measured electron backscatter diffraction patterns,” *Acta Mater.* **170**, 118–131.
- S. Shi, K. Zhou, J. Zhao, S. Mukherjee, and P. Zhuang (2021), “Heavy Quark Potential in QGP: DNN meets LQCD,” [arXiv:2105.07862 \[hep-ph\]](https://arxiv.org/abs/2105.07862).
- H. Shimodaira (2000), “Improving predictive inference under covariate shift by weighting the log-likelihood function,” *J. Stat. Plan. Inference* **90** (2), 227–244.
- E. Shintani, R. Arthur, T. Blum, T. Izubuchi, C. Jung, and C. Lehner (2015), “Covariant approximation averaging,” *Phys. Rev. D* **91** (11), 114511.
- J. Snoek, H. Larochelle, and R. P. Adams ((2012)), “Practical bayesian optimization of machine learning algorithms,” in *Adv. Neural Inf. Process. Syst.*, pp. 2951–2959, [arXiv:1206.2944 \[stat.ML\]](https://arxiv.org/abs/1206.2944).
- R. Solli, D. Bazin, M. Hjorth-Jensen, M. P. Kuchera, and R. R. Strauss (2021), “Unsupervised learning for identifying events in active target experiments,” *Nucl. Instrum. Methods Phys. Res. A* **1008**, 165461.
- A. Solopova, A. Carpenter, T. Powers, Y. Roblin, C. Tennant, L. Vidyaratne, and K. Iftekharuddin (2019), “Srf cavity fault classification using machine learning at CEBAF,” in *10th Int. Particle Accelerator Conf.(IPAC’19), Melbourne, Australia, 19-24 May 2019* (JACOW Publishing, Geneva, Switzerland) pp. 1167–1170.
- D. L. B. Sombillo, Y. Ikeda, T. Sato, and A. Hosaka (2020), “Classifying the pole of an amplitude using a deep neural network,” *Phys. Rev. D* **102**, 016024.
- D. L. B. Sombillo, Y. Ikeda, T. Sato, and A. Hosaka (2021a), “Classifying near-threshold enhancement using deep neural network,” *Few-Body Syst.* **62** (3), 52.
- D. L. B. Sombillo, Y. Ikeda, T. Sato, and A. Hosaka (2021b), “Unveiling the pole structure of S-matrix using deep learning,” [arXiv:2104.14182 \[hep-ph\]](https://arxiv.org/abs/2104.14182).
- C. Soto (2019), “Visual detection with context for document layout analysis,” in *Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP)* (Association for Computational Linguistics, Hong Kong, China) p. 3464.
- T. M. Sprouse, R. Navarro Perez, R. Surman, M. R. Mumpower, G. C. McLaughlin, and N. Schunck (2020), “Propagation of statistical uncertainties of Skyrme mass models to simulations of r -process nucleosynthesis,” *Phys. Rev. C* **101**, 055803.
- J. Steinheimer, L. Pang, K. Zhou, V. Koch, J. Randrup, and H. Stoecker (2019), “A machine learning study to identify spinodal clumping in high energy nuclear collisions,” *JHEP* **12**, 122.
- R. Stevens, V. Taylor, J. Nichols, A. B. Maccabe, K. Yelick, and D. Brown (2020), *AI for Science*, Tech. Rep. (Argonne National Lab. (ANL), Argonne, IL (United States)).
- M. Sugiyama, and M. Kawanabe (2012), *Machine learning in non-stationary environments: Introduction to covariate shift adaptation* (MIT press).
- R. S. Sutton, and A. G. Barto (2018), *Reinforcement learning: An introduction* (MIT press).
- I. Svensson, A. Ekström, and C. Forssén (2021), “Bayesian parameter estimation in χ EFT using Hamiltonian Monte Carlo,” [arXiv:2110.04011 \[nucl-th\]](https://arxiv.org/abs/2110.04011).
- S.-P. Tang, J.-L. Jiang, M.-Z. Han, Y.-Z. Fan, and D.-M. Wei (2021), “Constraints on the phase transition and nuclear symmetry parameters from PSR J0740 + 6620 and multimessenger data of other neutron stars,” *Phys. Rev. D* **104**, 063032.
- C. Tennant, A. Carpenter, T. Powers, A. Shabalina Solopova, L. Vidyaratne, and K. Iftekharuddin (2020), “Supercon-

- ducting radio-frequency cavity fault classification using machine learning at jefferson laboratory,” *Phys. Rev. Accel. Beams* **23**, 114601.
- A. Tomiya, and Y. Nagai (2021), “Gauge covariant neural network for 4 dimensional non-abelian gauge theory,” [arXiv:2103.11965 \[hep-lat\]](https://arxiv.org/abs/2103.11965).
- J. Townsend, and K. D. Vogiatzis (2020), “Transferable MP2-based machine learning for accurate coupled-cluster energies,” *J. Chem. Theory Comput.* **16** (12), 7453–7461.
- C. Tsang, M. Tsang, P. Danielewicz, F. Fattoyev, and W. Lynch (2019), “Insights on Skyrme parameters from GW170817,” *Phys. Lett. B* **796**, 1 – 5.
- V. Tshitoyan, *et al.* (2019), “Unsupervised word embeddings capture latent knowledge from materials science literature,” *Nature* **571**, 95–98.
- R. Utama, W. C. Chen, and J. Piekarewicz (2016a), “Nuclear charge radii: density functional theory meets Bayesian neural networks,” *J. Phys. G* **43**, 114002.
- R. Utama, and J. Piekarewicz (2017), “Refining mass formulas for astrophysical applications: A Bayesian neural network approach,” *Phys. Rev. C* **96**, 044308.
- R. Utama, and J. Piekarewicz (2018), “Validating neural-network refinements of nuclear mass models,” *Phys. Rev. C* **97**, 014306.
- R. Utama, J. Piekarewicz, and H. B. Prosper (2016b), “Nuclear mass predictions for the crustal composition of neutron stars: A Bayesian neural network approach,” *Phys. Rev. C* **93**, 014311.
- I. Vernon, M. Goldstein, and R. Bower (2014), “Galaxy Formation: Bayesian History Matching for the Observable Universe,” *Statist. Sci.* **29** (1), 81 – 90.
- V. Vigneron, J. Morel, M. Lépy, and J. Martinez (1996), “Statistical modelling of neural networks in γ -spectrometry,” *Nucl. Instrum. Methods Phys. Res. A* **369** (2), 642–647.
- R. Wang, Y.-G. Ma, R. Wada, L.-W. Chen, W.-B. He, H.-L. Liu, and K.-J. Sun (2020), “Nuclear liquid-gas phase transition with machine learning,” *Phys. Rev. Research* **2**, 043202.
- Z.-A. Wang, J. Pei, Y. Liu, and Y. Qiang (2019), “Bayesian evaluation of incomplete fission yields,” *Phys. Rev. Lett.* **123**, 122501.
- Z. A. Wang, J. C. Pei, Y. J. Chen, C. Y. Qiao, F. R. Xu, Z. G. Ge, and N. C. Shu (2021), “Bayesian data fusion of imperfect fission yields for augmented evaluations,” [arXiv:2111.14102 \[nucl-th\]](https://arxiv.org/abs/2111.14102).
- S. Wesolowski, R. J. Furnstahl, J. A. Melendez, and D. R. Phillips (2019), “Exploring Bayesian parameter estimation for chiral effective field theory using nucleon–nucleon phase shifts,” *J. Phys. G* **46** (4), 045102.
- S. Wesolowski, I. Svensson, A. Ekström, C. Forssén, R. J. Furnstahl, J. A. Melendez, and D. R. Phillips (2021), “Rigorous constraints on three-nucleon forces in chiral effective field theory from fast and accurate calculations of few-body observables,” *Phys. Rev. C* .
- S. J. Wetzel, and M. Scherzer (2017), “Machine Learning of Explicit Order Parameters: From the Ising Model to SU(2) Lattice Gauge Theory,” *Phys. Rev. B* **96** (18), 184410, [arXiv:1705.05582 \[cond-mat.stat-mech\]](https://arxiv.org/abs/1705.05582).
- B. Whewell, M. Grosskopf, and D. Neudecker (2020), “Evaluating $^{239}\text{Pu}(\text{n},\text{f})$ cross sections via machine learning using experimental data, covariances, and measurement features,” *Nucl. Instrum. Methods Phys. Res. A* **978**, 10.1016/j.nima.2020.164305.
- D. M. Wilkins, A. Grisafi, Y. Yang, K. U. Lao, R. A. DiStasio, and M. Ceriotti (2019), “Accurate molecular polarizabilities with coupled cluster theory and machine learning,” *PNAS* **116** (9), 3401–3406.
- C. Williams, and C. Rasmussen (1996), “Gaussian processes for regression,” in *Adv. Neural Inf. Process. Syst.*, Vol. 8, edited by D. Touretzky, M. C. Mozer, and M. Hasselmo (MIT Press).
- D. Wu, C. L. Bai, H. Sagawa, S. Nishimura, and H. Q. Zhang (2021a), “ β -delayed one-neutron emission probabilities within a neural network model,” *Phys. Rev. C* **104**, 054303.
- D. Wu, C. L. Bai, H. Sagawa, and H. Q. Zhang (2020), “Calculation of nuclear charge radii with a trained feed-forward neural network,” *Phys. Rev. C* **102**, 054323.
- X. H. Wu, L. H. Guo, and P. W. Zhao (2021b), “Nuclear masses in extended kernel ridge regression with odd-even effects,” *Phys. Lett. B* **819**, 136387.
- X. H. Wu, and P. W. Zhao (2020), “Predicting nuclear masses with the kernel ridge regression,” *Phys. Rev. C* **101**, 051301.
- J.-L. Wynen, E. Berkowitz, S. Krieg, T. Luu, and J. Ostheimer (2021), “Machine learning to alleviate Hubbard-model sign problems,” *Phys. Rev. B* **103** (12), 125153.
- W.-J. Xie, and B.-A. Li (2020), “Bayesian inference of the symmetry energy of superdense neutron-rich matter from future radius measurements of massive neutron stars,” *AJ* **899** (1), 4.
- W.-J. Xie, and B.-A. Li (2021), “Bayesian inference of the incompressibility, skewness and kurtosis of nuclear matter from empirical pressures in relativistic heavy-ion collisions,” *J. Phys. G* **48** (2), 025110.
- J. Xu, W.-J. Xie, and B.-A. Li (2020), “Bayesian inference of nuclear symmetry energy from measured and imagined neutron skin thickness in $^{116,118,120,122,124,130,132}\text{Sn}$, ^{208}Pb , and ^{48}Ca ,” *Phys. Rev. C* **102**, 044316.
- Y. Xu, J. E. Bernhard, S. A. Bass, M. Nahrgang, and S. Cao (2018), “Data-driven analysis for the temperature and momentum dependence of the heavy-quark diffusion coefficient in relativistic heavy-ion collisions,” *Phys. Rev. C* **97** (1), 014907.
- J. Yang, and J. Piekarewicz (2020), “Covariant density functional theory in nuclear physics and astrophysics,” *Ann. Rev. Nucl. Part. Sci.* **70** (1), 21–41.
- L. Yang, C. Lin, Y. Zhang, P. Wen, H. Jia, D. Wang, N. Ma, F. Yang, F. Zhong, S. Zhong, and T. Luo (2020), “Bayesian analysis on interactions of exotic nuclear systems,” *Phys. Lett. B* **807**, 135540.
- X. Ye, H. Jian, and Z. Kai-En (2008), “Applying Bayesian neural networks to identify pion, kaon and proton in BE-SII,” *Chin. Phys. C* **32** (3), 201–204.
- B. Yoon, T. Bhattacharya, and R. Gupta (2019), “Machine learning estimators for lattice qcd observables,” *Phys. Rev. D* **100**, 014504.
- S. Yoshida (2020), “Nonparametric Bayesian approach to extrapolation problems in configuration interaction methods,” *Phys. Rev. C* **102**, 024305.
- S. Yoshida, and N. Shimizu (2021), “A new workflow of shell-model calculations with the emulator and preprocessing using eigenvector continuation, and shell-model code ShellModel.jl,” [arXiv:2105.08256 \[nucl-th\]](https://arxiv.org/abs/2105.08256).
- S. Yoshida, N. Shimizu, T. Togashi, and T. Otsuka (2018), “Uncertainty quantification in the nuclear shell model,” *Phys. Rev. C* **98**, 061301.
- Y.-Z. You, Z. Yang, and X.-L. Qi (2018), “Machine Learn-

- ing Spatial Geometry from Entanglement Features,” *Phys. Rev. B* **97** (4), 045153, arXiv:1709.01223 [cond-mat.dis-nn].
- E. Yüksel, D. Soydane, and H. Bahtiyar (2021), “Nuclear binding energy predictions using neural networks: Application of the multilayer perceptron,” *Int. J. Mod. Phys. E* **30** (03), 2150017.
- M. D. Zeiler, D. Krishnan, G. W. Taylor, and R. Fergus (2010), “Deconvolutional networks,” in *Proc. IEEE Comput. Soc. Conf. Comput. Vis. Pattern Recognit.* (IEEE) pp. 2528–2535.
- R. Zhang, Z. Fan, R. Li, H.-W. Lin, and B. Yoon (2020a), “Machine-learning prediction for quasiparton distribution function matrix elements,” *Phys. Rev. D* **101** (3), 034516, arXiv:1909.10990 [hep-lat].
- X. Zhang, and R. J. Furnstahl (2021), “Fast emulation of quantum three-body scattering,” arXiv:2110.04269 [nucl-th].
- X. Zhang, K. M. Nollett, and D. R. Phillips (2020b), “S-factor and scattering-parameter extractions from $^3\text{He} + ^4\text{He} \rightarrow ^7\text{Be} + \gamma$,” *J. Phys. G* **47** (5), 054002.
- X. Zhang, *et al.* (2021a), “Determining impact parameters of heavy-ion collisions at low-intermediate incident energies using deep learning with convolutional neural network,” arXiv:2111.06597 [nucl-th].
- Y. Zhang, and Q. Yang (2021), “A survey on multi-task learning,” arXiv:1707.08114 [cs.LG].
- Z. Zhang, X.-B. Feng, and L.-W. Chen (2021b), “Bayesian inference on isospin splitting of nucleon effective mass from giant resonances in ^{208}Pb ,” *Chin. Phys. C* **45** (6), 064104.
- Y.-S. Zhao, L. Wang, K. Zhou, and X.-G. Huang (2021), “Detecting Chiral Magnetic Effect via Deep Learning,” arXiv:2105.13761 [hep-ph].
- J. Zhu, Y. Chen, F. Brinker, W. Decking, S. Tomin, and H. Schlarb (2021), “Deep learning-based autoencoder for data-driven modeling of an RF photoinjector,” arXiv preprint arXiv:2101.10437 .