Machine Learning and Artificial Intelligence activities at FRIB

Contents

1 Explanation

The purpose of this living document is to collect information about the competence in the area of ML/AI at FRIB Laboratory. This material was used to inform *AI for Nuclear Physics Workshop* at JLab, March 4-6, 2020 (see report); and *Workshop for Applied Nuclear Data Activities* at George Washington University, March 3-5, 2020; and other related activities.

1.1 Description of individual entries

Please format your entry (1 entry per page) according to the following template:

> **Topic** (in subsubsection title. Capitalize words)
>
> **Participants** List local faculty/staff, research associates (p), students (g,u). External collaborators should be listed as co-authors in references.
>
> **Description** Provide a short paragraph (<600 characters; think of a PRL abstract) describing the ML/AI aspects of the project. To provide uniformity, use the acronyms defined in Sec. 2.2
>
> **FRIB relevance** (<600 characters)
>
> **Outcomes** List instrumentation outcomes, if any. Provide your published/submitted/anticipated papers with **hyperlinks**.
>
> You are encouraged to provide a figure below the description. If needed, use side captions as in entry 3.1.3.

2 Machine Learning and AI in Nuclear Physics

Artificial intelligence (AI)-based techniques, particularly in machine learning (ML) and optimization, are increasingly being used in many areas of experimental and theoretical physics to facilitate discovery, accelerate data analysis and modeling efforts, and bridge different physical and temporal scales in numerical models. The large amount of degrees of freedom pertain to both theory and experiment in nuclear physics. With increasingly complicated experiments that produce large amounts data, automated classification of events becomes increasingly important. Artificial intelligence and Machine Learning techniques are proving to be powerful tools for advancing our understanding of the physics from complicated nuclear systems.

2.1 Types of Machine Learning

The approaches to machine learning are many, but are often split into two main categories. In *supervised learning* we have a situation with known input and output data that we want to reproduce with a given set of models, letting the given machine learning algorithm deduce the eventual logic behind our data.

On the other hand, *unsupervised learning* is a method for finding patterns and relationship in data sets without any prior knowledge of the system. Some authors also operate with a third category, namely *reinforcement learning*. This is a paradigm of learning inspired by behavioural psychology, where learning is achieved by trial-and-error, solely from rewards and punishment.

Some of the most common tasks are:

- 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 ones.
- Regression: Finding a functional relationship between an input data set and a reference data set. The goal is to construct a function that maps input data to continuous output values.
- Clustering: Data are divided into groups with certain common traits, without knowing the different groups beforehand. It is thus a form of unsupervised learning.

These categories are all part of the broad spectrum of AI and ML techniques being studied at FRIB.

2.2 Acronyms of machine learning/statistical terms used

We list here various acronyms used in the description of the different AI/ML projects.

AE Auto encoders

AI Artificial intelligence

ANN Artificial neural networks

BC Bayesian calibration

BM Boltzmann machines

BMA Bayesian model averaging

BML Bayesian machine learning

BNN Bayesian neural networks

BS Bayesian statistics

CI Credibility interval

CL Clustering

CNN Convolutional neural networks

CoD Coefficient of determination

DL Deep learning

DRB Decision trees, random forests and boosting

ECP Empirical coverage probability

FS Frequentist statistics

GM Graphical models

GP Bayesian Gaussian processes

KR Kernel regression

LR Logistic regression

LSTM Long short-term memory

MCMC Markov chain Monte Carlo

ML Machine learning

NN Neural networks

PCA Principal component analysis and dimensionality reduction techniques

REG Linear regression

RL Reinforcement learning

RNN Recurrent neural networks

SL Supervised learning

SVM Support vector machines

UQ Uncertainty quantification

VAE Variational auto encoders

3 AI/ML projects at FRIB

3.1 Accelerators/Beam Tuning

3.1.1 Artificial Intelligence Aided Beam Tuning

Participants: Y.Hao, S.Lidia, T.Maruta, L.Neufcourt(p), A.Plastun and T.Zhang

Description: The capability of providing versatile species of ions presents a challenge of fast accelerator tuning of the new ion species to maintain the high availability of scientific discoveries. The recent progress on AI shines a light on a new approach to achieve fast tuning. We propose to establish a data-refined accelerator model for fast tuning using AI based on the existing diagnostic data. The proposed work including the inference of parameters in the accelerator model and creating a surrogate model using the GP or ANN for the components that cannot be well predicted by physics model.

FRIB relevance: The ML and BS application in Beam tuning provide new methods to quickly switch the operation modes of FRIB.

Outcomes: *Y. Hao and L. M. Neufcourt, "Application of Bayesian Inference in Accelerator Commissioning of FRIB", in Proc. 10th Int. Particle Accelerator Conf. (IPAC'19), Melbourne, Australia, May 2019*

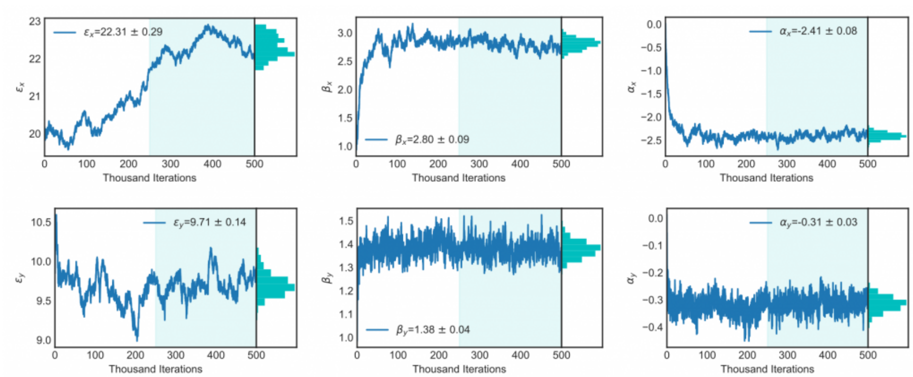

Figure 1: The iterations of inferring the beam linear properties at the exit of the ion source using Bayesian Inference

3.1.2 Beam loss Control and Machine Protection with Artificial Intelligence

Participants: Y.Hao, S.Lidia, L.Neufcourt(p) and T.Zhang

Description: The beam loss control and high-fidelity machine protection system are essential tasks to achieve the 400 KW ion beam power in FRIB. Artificial intelligence provides a powerful toolset in predicting and localizing the beam loss, anomaly detection and unloading the risk of the hardware damage due to beam loss. We propose to create a surrogate model with GP or ANN to identify the correlation of beam properties and the beam loss using diagnostic data from BPMs and loss monitors, 'forecast' and prevent the hardware damage due to excess power from beam loss.

FRIB relevance: The surrogate model create by AI may largely protect the accelerator from damaging or degrading due to beam losses and improve the availability of the accelerator.

Outcomes: *None*

3.1.3 Machine learning SECAR tuning optimization

Participants F. Montes, H. Schatz, K. Hermansen (g), S. Ayoub (g), D. Crisp, T. Summers and A.M. Amthor (Bucknell)

Description The primary purpose of the The SEparator for CApture Reactions (SECAR) at FRIB is to measure resonance strengths in radiative proton and alpha capture reactions for astrophysics. We have developed and tested systems to interpret data in real-time from existing spectrometer and beam-line systems to tune multiple elements to provide desired beam properties without providing the autonomous system a theoretical model of the particle-optical system being tuned. Preliminary SECAR optimization simulations have shown that such a technique can also be used to produce an achromatic dispersive image in SECAR by using autonomous optimization approaches such as a GP, NN and/or the Particle Swarm method. We are now working toward a further test of the automated optimization to independently minimize the beam-spot size at different critical positions in SECAR, thus maximizing beam purity and mass resolving power, which are critical to maximizing the scientific productivity of SECAR.

FRIB relevance Automated optimization is expected to reduce tuning time and improve quality and consistency of SECAR performance. These techniques are also applicable to other FRIB accelerator, beam-line, and spectrometer systems.

Outcomes: *Experimental test of an online ion-optics optimizer, Amthor A. M., Schillaci Z. M., Morrissey D. J., Portillo M., Schwarz S., Steiner M., Sumithrarachchi C.* Nuc. Inst. and Meth. in Phys. Res. A, 895, 90 (2018)

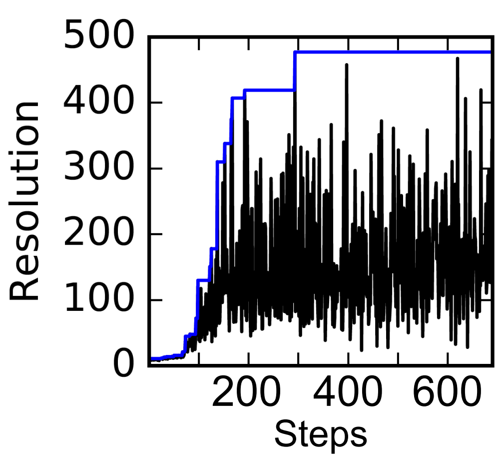

Figure 2: SECAR mass resolution as a function of the number steps in the optimization. Each step corresponds to a different optics configuration.

3.2 Detectors

3.2.1 Gamma-ray Tracking

Participants: D. Weisshaar, A. Gade, L. Neufcourt, J. Chung

Description: Gamma-ray tracking algorithms determine how many γ rays got fully or partially absorbed in an event by analyzing the measured interaction positions and energy depositions. Experimental energy measurements and computer simulations can constitute a large set of data on which ML models such as neural networks can be trained to identify patterns in interaction points. This approach does make no assumption about the underlying scattering processes (Compton scatter, Photo effect, pair production) as state-of-the-art deterministic algorithms do, especially the handling of wrongly reported interaction points by the detectors.

FRIB relevance: The Gamma-Ray Energy Tracking Array GRETA will be one of the premium devices at FRIB. Improvement on its tracking capability in terms of better identification of incomplete absorbed γ rays will directly translate into better spectral quality and sensitivity of this device, enlarging its scientific reach.

Outcomes: none

Figure 3: To be added

3.3 Data Analysis and Statistical Analysis

3.3.1 Machine learning methods for track classification in the AT-TPC

Participants: D. Bazin, M. Hjorth-Jensen

Description: We have implemented several ML methods for event classification in the Active-Target Time Projection Chamber (AT-TPC) detector at NSCL. In particular we have implemented advanced convolutional AE NN to the analysis of two-dimensional projections of particle tracks from a resonant proton scattering experiment on ^{46}Ar.

FRIB relevance: We expect that many of the new FRIB experiments will produce large amounts of data. A class of detectors such as the AT-TPC is able to detect several reaction channels simultaneously. Extracting low cross section channels requires to classify the events of interest, which requires a large degree of automation. We expect that these techniques will play a central role at FRIB.

Outcomes: *Machine learning methods for track classification in the AT-TPC*, M.P.Kuchera, R.Ramanujan, J.Z.Taylor, R.R.Strauss, D.Bazin, J.Bradt, R.M. Chen, Nucl. Inst. Meth. A 940, 56 (2019)

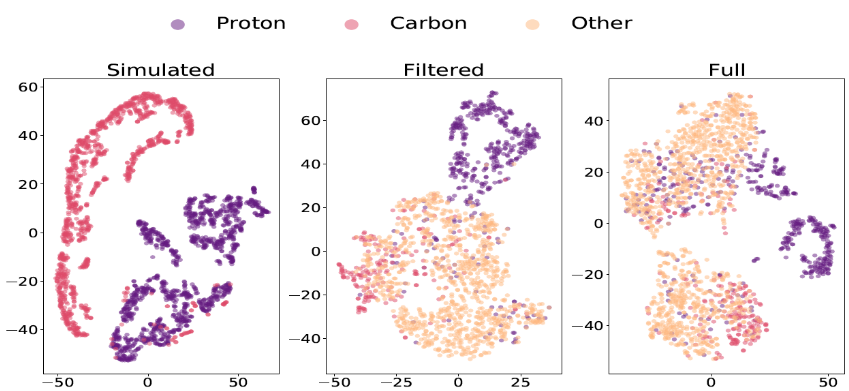

Figure 4: Visualization of the latent space from the VGG16 model on three different data-sets. The axes have arbitrary non-informative units.

3.3.2 Machine learning methods for multi-hit identification in time and/or space

Participants: P. Johns (u), G. T. Ulvik (g), S. N. Liddick, M. Hjorth-Jensen

Description: Shape coexistence is a phenomenon in which promotion of nucleons across an energy gap can become energetically favored and coexist at low-excitation energies with standard shell model configurations. Shape coexistence can be sensitively studied following the population of specific states in beta decay that subsequently undergo E0 electromagnetic transitions. Such transitions are forbidden to proceed through gamma-ray emission and instead occur through the emission of an internal conversion electron. The resulting experimental signature is the emission of two electrons.

We have used, with success, various classification methods to distinguish between various electron processes, in particular CNNs, AEs, RNNSs and VAEs to to distinguish between one and two electron events and predict the electron(s) corresponding initial position(s) and energies.

FRIB relevance: We expect that many of the new FRIB experiments will produce large amounts of data with loose triggering conditions that can be used to achieve multiple high-impact results for each experiment. The techniques developed here will enable access to scientific outcomes that are difficult or impossible with current technology.

Outcomes: In preparation

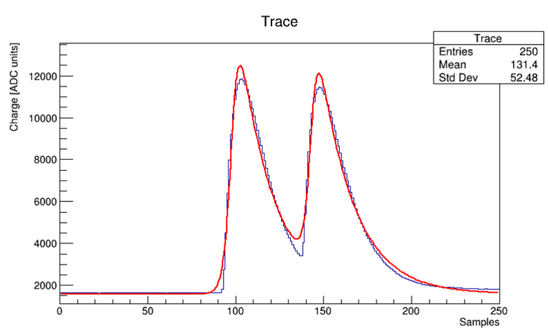

Figure 5: Example of a waveform with multiple pulses in a single detector element. Black is the experimental voltage as a function of time and red is the currently used analytical fit. Each sample is 2 nanoseconds. AI methods could be used to improve the classification of waveforms leading to better identification of multiple pulses and extracting the energy of each pulse and their relative time separation

3.3.3 Machine learning methods for detector response removal following beta decay

Participants: C. Dembsky (u), C. Arbour (u), S. N. Liddick, S. Spyrou, M. Hjorth-Jensen

Description: The technique of total absorption spectroscopy was developed more than 30 years ago to provide an accurate measurement of the beta-decay feeding into different excitation energies of the nucleus. The beta-decay feeding intensity is a sensitive probe to study the structure of the nucleus as it has different distributions depending on the shape of the nucleus of interest. The feeding intensity is also critical in a number of applications ranging from astrophysics to national security. The response of a large volume gamma-ray total absorption spectrometer is complex and depends sensitively on the excitation energy, the individual gamma-ray energies, and the gamma-ray multiplicity. The application of machine learning could greatly impact the accuracy and speed of extracting scientific insight from experimental data.

FRIB relevance: Total absorption experiments at FRIB will play a significant role in the beta-decay program. The application of machine learning could greatly impact the accuracy and speed of extracting scientific insight from experimental data. Once demonstrated, the technique could be extended to other experimental systems with lower efficiencies and higher energy resolutions.

Outcomes: In preparation.

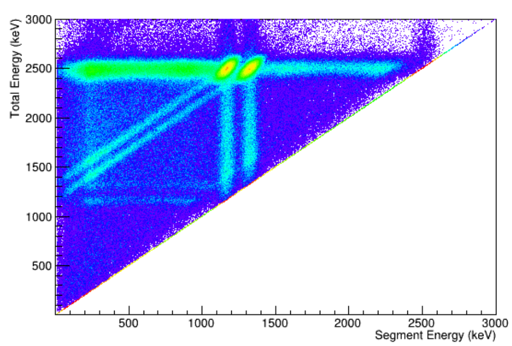

Figure 6: Spectrum of total energy deposited into SuN as a function of the energy deposited into individual segments following the decay of 60Co. AI methods could be used to remove the detector response from the experimentally recorded spectrum.

3.3.4 Particle identifications in radiation detectors

Participants: T. Ladourceur (u), C.Y. Tsang (g), W.G. Lynch, M.B. Tsang

Description: In nuclear collisions, physics information is obtained from emitted charged particles measured with radiation detectors. Identification of the emitted particles (PID) can be obtained from plotting the energy loss vs. total energy or momentum) as shown in the left panel of the figure. The data was obtained from SπRIT Time Projection Chamber. We test the ML algorithm using Monte Carlo events (right panel) from the TPC. A fully connected, feedforward NN classifier is used to separate out the various reaction products from simulated SπRIT data. Initially, we achieved an accuracy of 88%. However, with background tuning, we now achieve 97%, 92%, 85%, 77% and 88% for π, p, d, t, ^{3}He and α particles respectively. We plan to train and tune the algorithm with real data. We will extend the method to identify the PID lines constructed from data taken with the NSCL High Resolution Array (HiRA).

FRIB relevance: PID lines are ubiquitous observable in nearly all nuclear physics experiments that detect charged particles. ML tools and strategies will be needed for fast particle identifications to facilitate the huge amount of data from FRIB experiments.

Outcomes: *Non-linearity effects on the light-output calibration of light charged particles in CsI(Tl) scintillator crystals*, D. Dell'Aquila, S. Sweany, et al., Nucl. Instrum. Methods Phys. Res. A 929 (2019) 162-172.

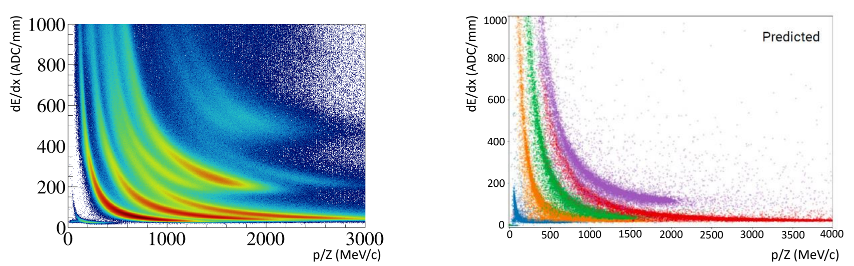

Figure 7: (left panel) Particle identifications from ^{132}Sn+^{124}Sn collisions at 270 MeV/u measured with the SπRIT TPC. (Right panel). Particle identifications from Monte Carlo events using Machine learning for π^+, p, d, t, ^{3}He.

3.4 Basic Research

3.4.1 Bayesian Approach to Extrapolations of Nuclear Observables

Participants: L. Neufcourt (p), Y. Cao (s), W. Nazarewicz, and F. Viens (STT)

Description: To improve the quality of model-based predictions of nuclear properties of rare isotopes far from stability, we consider the information contained in the residuals in the regions where the experimental information exist. The emulators of residuals and CIs defining theoretical error bars are constructed using GP and BNN.

FRIB relevance: The proposed Bayesian SL approach to extrapolation of nuclear model predictions can be useful for assessing the impact of current and future FRIB experiments. The new capability to evaluate residuals is also expected to impact research in the domains where experiments are currently impossible, for instance, in simulations of the astrophysical r process.

Outcomes: *Bayesian approach to model-based extrapolation of nuclear observables*, L. Neufcourt, Y. Cao, W. Nazarewicz, and F. Viens, Phys. Rev. C 98, 034318 (2018) (Editor's Suggestion).

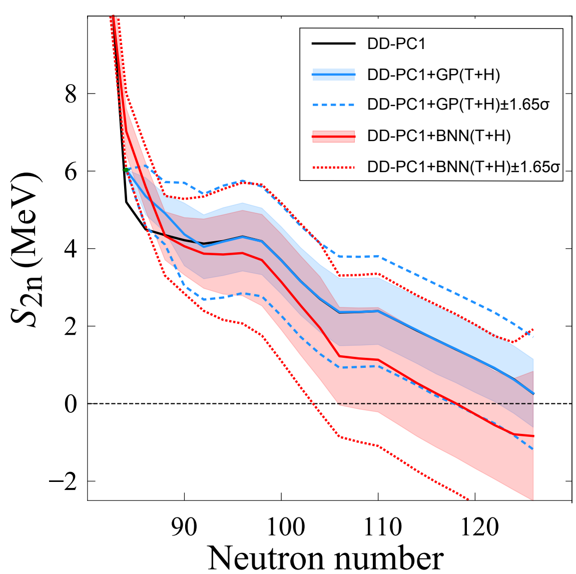

Figure 8: Extrapolations of two-neutron separation energies for the even-even Sn chain calculated with DD-PC1 model with statistical GP and BNN approaches. One-sigma and 1.65-sigma CIs are marked.

3.4.2 Nuclear Landscape with Bayesian Model Averaging

Participants: L. Neufcourt (p), Y. Cao (g), S.A. Giuliani (p), W. Nazarewicz, F. Viens (STT), and O.B. Tarasov

Description: We use microscopic nuclear global mass models and Bayesian SL methodology to provide quantified predictions of proton and neutron separation energies as well as Bayesian probabilities of existence throughout the nuclear landscape all the way to the particle drip lines. To account for uncertainties, Bayesian GP are trained on the separation-energy residuals for each individual model, and the resulting predictions are combined via BMA. This framework allows to account for systematic and statistical uncertainties and propagate them to extrapolative predictions.

FRIB relevance: Considering the anticipated FRIB production rates and uncertainties of theoretical predictions, we identified regions, reached by FRIB, that are crucial for constraining theoretical mass models.

Outcomes: *Neutron Drip Line in the Ca Region from Bayesian Model Averaging*, Phys. Rev. Lett. 122, 062502 (2019); *Beyond the proton drip line: Bayesian analysis of proton-emitting nuclei*, Phys. Rev. C 101, 014319 (2020); *Quantified limits of the nuclear landscape*, Phys. Rev. C 101, 044307 (2020). L. Neufcourt, Y. Cao, S. Giuliani, W. Nazarewicz, E. Olsen, F. Viens,and O.B. Tarasov

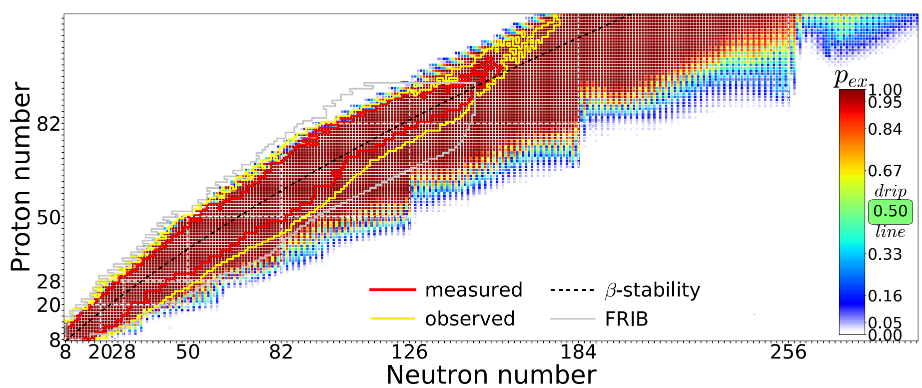

Figure 9: The quantified landscape of nuclear existence obtained in our BMA calculations. For every nucleus with $Z, N \geq 8$ and $Z \leq 119$ the probability that the nucleus is bound with respect to proton and neutron decay, is marked. The domains of nuclei which have been experimentally observed and whose separation energies have been measured (and used for training) are indicated together with the experimental reach of FRIB.

3.4.3 Statistical Aspects of Nuclear Mass Models

Participants: V. Kejzlar (g), L. Neufcourt (p), W. Nazarewicz, and P.-G. Reinhard (Erlangen)

Description: We study the information content of nuclear masses from the perspective of global models of nuclear binding energies. To this end, we employ a number of statistical methods and diagnostic tools, including BC, BMA, REG, PCA, and ECP by considering discrepant mass domains for calibration. We show that a quite dramatic parameter reduction can be achieved.

FRIB relevance: The use of statistical methodologies and diagnostic tools advocated in this work will be useful in further studies of nuclear models, both for the sake of understanding their structure and for practical applications pertaining to FRIB science.

Outcomes: *Statistical aspects of nuclear mass models*, V. Kejzlar L. Neufcourt, W. Nazarewicz, and P.-G. Reinhard, Submitted to the J. Phys. G Focus ISNET 2 Issue.

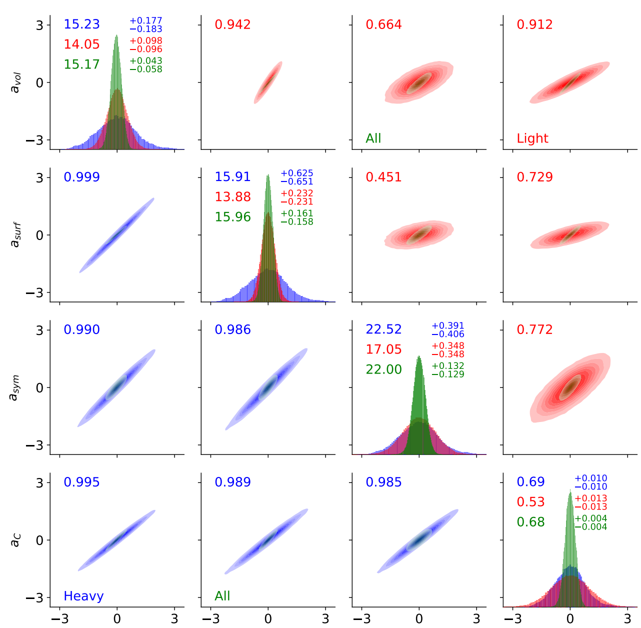

Figure 10: Posterior distribution of the parameters for three liquid drop model variants fitted on specific regions of the nuclear landscape. The conditioning data were the binding energies of even-even nuclei divided into light ($Z < 40$, $N < 50$), heavy ($Z > 50$, $N > 80$), and intermediate nuclei (remaining 155 nuclei). Posterior mean and standard deviation are indicated by numbers as well as correlation coefficients for all parameters.

3.4.4 Deep Learning and the Nuclear Many-Body Problem

Participants: J. Hartley (g), J. Kim (g), O. Udiani (g), S. Bogner, H. Hergert, and M Hjorth-Jensen

Description: ML methods make it possible to tackle the curse of dimensionality and allow us to model quantum mechanical systems with less a priori knowledge. For complex many-body systems like nuclei (especially those at the limits of stability) or nuclear matter, this is a very interesting avenue to explore. We have recently applied DL methods — particular RNNs, LSTM and KRR — to Similarity Renormalization Group flows and the solution of Coupled Cluster theory, with a great deal of success. Our preliminary studies hold great promise for handling systems with large numbers of particles (including nuclear matter) or basis states (e.g. due to deformation or continuum coupling).

FRIB relevance: Theoretical studies of nuclei at the limits of stability are a great challenge due to the large number of degrees of freedom. These systems are highly relevant for the scientific program of FRIB. Our early results also suggest connections between RG methods and Deep Learning that will contribute to a better understanding of Machine Learning methods.

Outcomes: *Recurrent Neural Networks and the Nuclear Many-body Problem*, in preparation

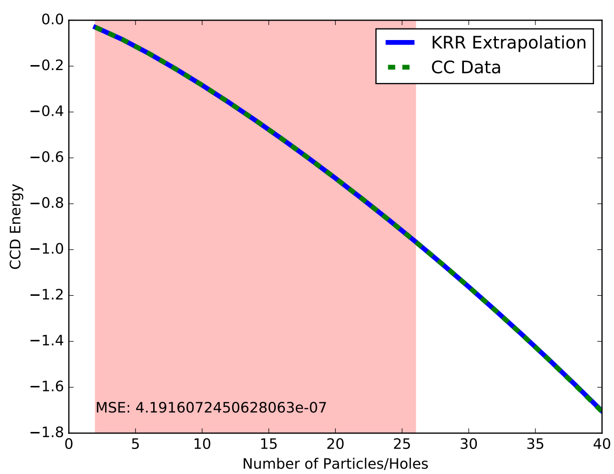

Figure 11: Extrapolations to large numbers of interacting fermions for a pairing model using KRR methods on Coupled Cluster data.

3.4.5 Boltzmann Machines and the Nuclear Many-Body Problem

Participants: J. Hartley (g), J. Kim (g), S. Bogner, and M Hjorth-Jensen

Description: We have recently started to explore several approaches based on DL algorithms, with an emphasis on NN and BM, with several promising results for interacting many-fermion systems. Our applications so far have been to systems of electrons confined to move in two or three-dimensional regions (so-called quantum dots) and systems of bosons (weakly and strongly interacting) using a mix of NN based algorithms and variational quantum Monte Carlo approaches. We are in the process of extending these calculations to nuclear physics problems.

FRIB relevance: The ability to study theoretically nuclei at the limits of stability is a great challenge due to the huge number of degrees of freedom. These systems are highly relevant for the scientific program of FRIB.

Outcomes: *Solving Many-Body Problems with Boltzmann Machines*, in preparation

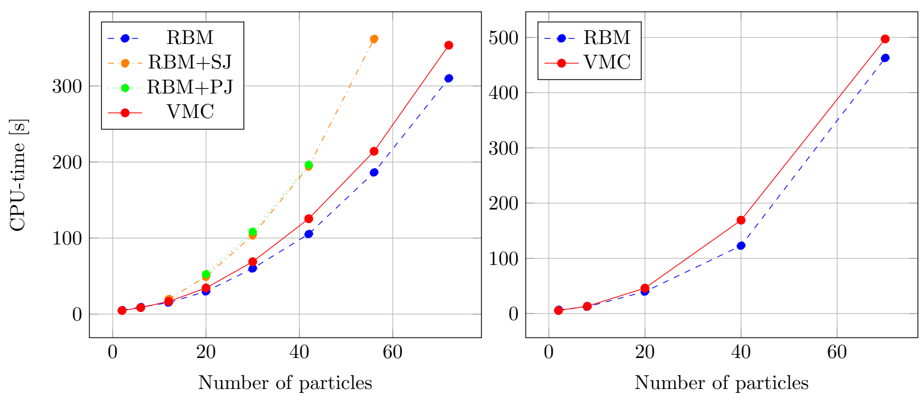

Figure 12: Ground state energies for systems of quantum dots.

3.4.6 Emulators for the Nuclear Many-Body Problem

Participants: D. Lee

Description: In applications of machine learning and uncertainty quantification to first principles nuclear many-body theory, one important tool is a fast and accurate emulator that removes the need for repeatedly performing computationally-expensive calculations. We show that eigenvector continuation can fill this role quite nicely. In addition to its applications as an emulator, eigenvector continuation can also be trained as a machine learning method for the quantum many-body problem using optimized variational subspaces.

FRIB relevance: One of the fundamental challenges in FRIB science is understanding the connection between microscopic nuclear forces and nuclear structure. Having a fast and accurate emulator makes it possible to apply machine learning and uncertainty quantification to uncover the correlations between nuclear forces and structure.

Outcomes: *Eigenvector Continuation as an Efficient and Accurate Emulator for Uncertainty Quantication in Nuclear Systems*, S. König, A. Ekström, K. Hebeler, D. Lee, and A. Schwenk, arXiv:1909.08446, submitted.

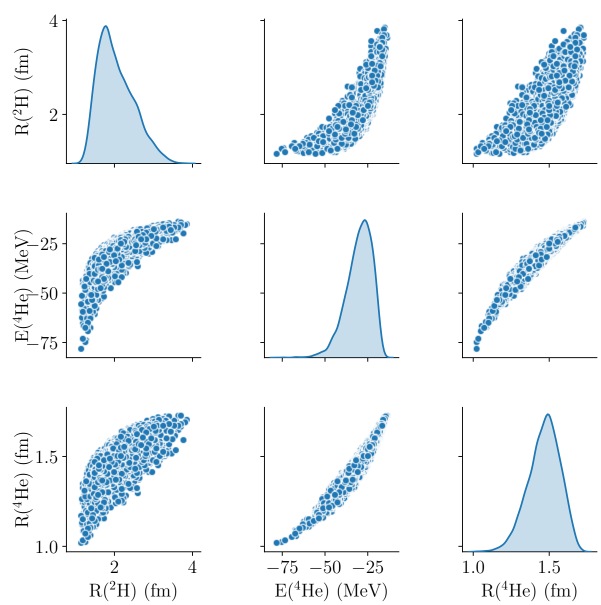

Figure 13: Correlations among several observables for ^{2}H and ^{4}He computed using eigenvector continuation.

3.4.7 Machine Learning Multi-Nucleon Correlations

Participants: J. Bonitati (g), G. Given (g), and D. Lee

Description: We are using BM to uncover and quantify multi-nucleon correlations in supercomputer lattice data obtained from lattice simulations of atomic nuclei. The work involves the development of new algorithms to bypass the computational bottleneck of computing the overall normalization of the partition function and dealing with negative weight configuration produced in the quantum simulations.

FRIB relevance: We would like to understand the microscopic origins of nuclear clustering across the nuclear chart. As the phenomenon of clustering is accentuated near open thresholds, these studies are of direct relevance to FRIB science.

Outcomes: *Machine Learning Multi-Nucleon Correlations from First Principles*, J. Bonitati, G. Given, Da. Lee, and D. Lee, in preparation.

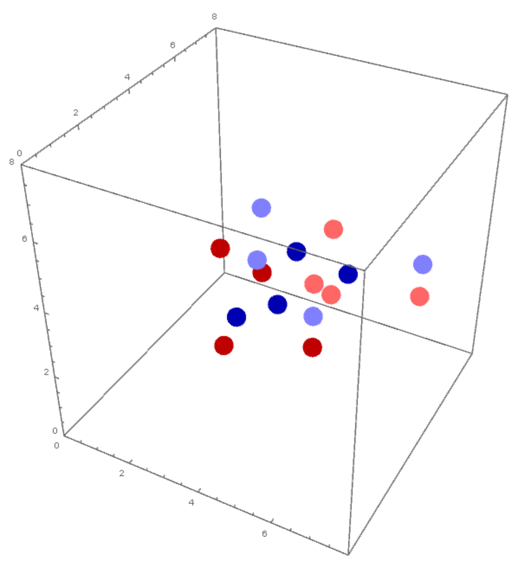

Figure 14: Sample training data used for machine learning multi-nucleon correlations in ^{16}O.

3.4.8 Machine Learning Algorithms for Hadron Correlators from Lattice QCD

Participants: G. Pederiva (g), A. Shindler

Description: Lattice QCD calculations are an effective tool to probe the dynamics of quarks and gluons at low energies. However, these calculations require large computational capabilities, for example when computing the building block of any hadron correlation function: the quark propagator. We are studying the feasibility of using ML, in particular algorithms based on Boosted Decision Trees and ANN, to reduce the cost of the iterative solvers for quark propagator by relating solutions to the system computed at different precision.

FRIB relevance: Understanding the nuclear structure starting from the strong interactions between quarks and gluons and between nucleons, is one of the main research thrusts of FRIB. Reducing the computational cost of quark propagator calculations could effectively lead to a precise determination of multi-nucleon correlators and nucleon scattering phase shifts with current state-of-the-art hardware and software.

Outcomes: *Machine Learning Algorithms for Hadron Correlators from Lattice QCD*, G. Pederiva, A. Shindler, in preparation

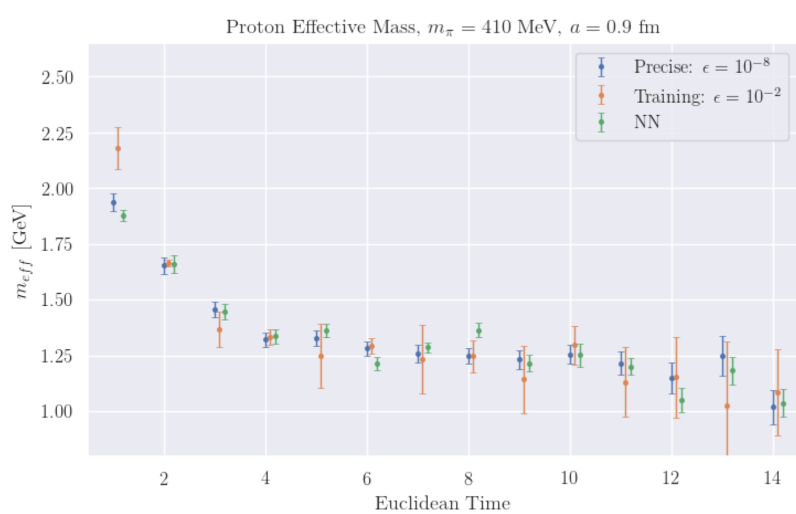

Figure 15: Example of proton effective mass plot with data from a precise calculation using a small stopping criterion $\epsilon = 10^{-8}$ in the BiCGStab solver, a training set using a much larger $\epsilon = 10^{-2}$, and the NN results for the same data.

3.4.9 Establishing a statistical approach to nuclear reactions

Participants: F.M. Nunes, A. Lovel (g), G. King (u), L. Neufcourt (p)

Description: The few-body group has been exploring statistical methods in nuclear reactions. In 2018 we compared, directly and systematically, the frequentist and Bayesian approaches to quantifying uncertainties in direct nuclear reactions. Our study demonstrated that the uncertainties on the reaction observables considered within the Bayesian approach represent reality more accurately than the much narrower uncertainties obtained using the standard frequentist approach.

FRIB relevance: To interpret reaction data from FRIB, we need to reliably quantify the uncertainties in the nuclear theories used.

Outcomes: G. B. King, A. E. Lovell, L. Neufcourt, and F. M. Nunes, Phys. Rev. Lett. 122, 232502 (2019).

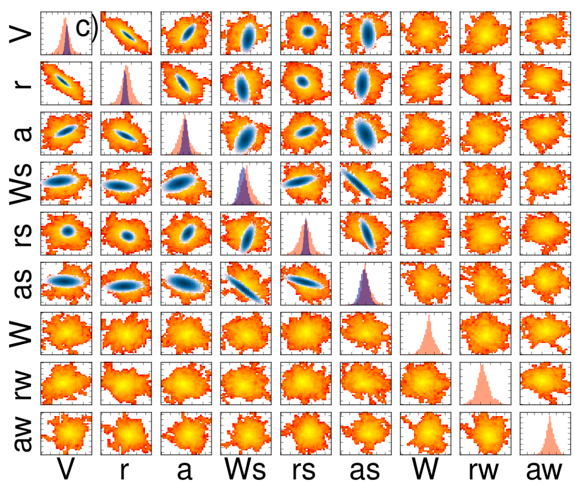

Figure 16: Posterior distributions for the parameters (diagonal) and scatter plots for the correlations between parameters: Bayesian are shown in shades of orange and frequentist in shades of blue for ^{48}Ca(p,p) at 25 MeV. Depths are in MeV and radii and difuseness are in fm.

3.4.10 Bayesian approach to nuclear reactions and Experimental Design

Participants: F.M. Nunes, A. Lovell (g), G. King (u) and M. Catacora-Rios (g)

Description: In recent work we study the uncertainties of optical model parameters and its dependence on the angular grid of the differential cross section, the inclusion of cross section data at nearby energies, and changes in the experimental error bars. We also study the effect on the resulting uncertainty when total reaction cross sections are included in the fitting procedure.

In the last years, we have been expanding our methods to include the PCA and BML to identify the optimum experimental conditions and the best combination of observables to reduce the uncertainty on the resulting cross sections. Once this is completed, we plan to use these statistical tools to make model comparisons and eventually, if it makes sense, to perform BMA

FRIB relevance: To plan reactions measurements at FRIB it is important to know what are the optimum conditions and the optimum observables (or combination of observables) that provide maximum information content.

Outcomes: M. Catacora-Rios, G. B. King, A. E. Lovell, and F. M. Nunes Phys. Rev. C 100, 064615 (2019).

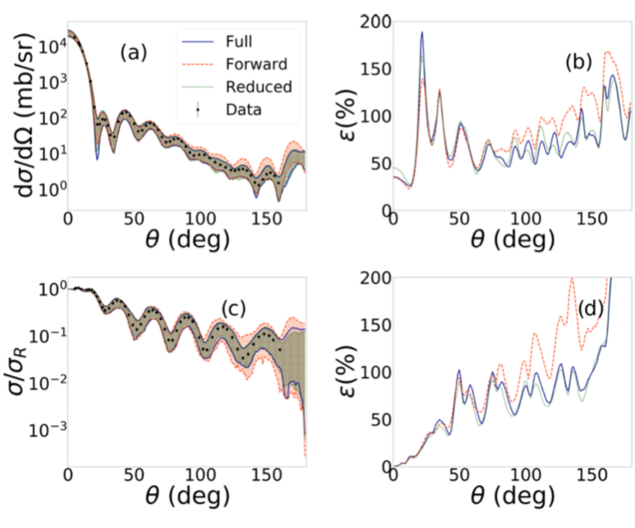

Figure 17: A comparison of results using the full angular range (blue solid line) with those where only forward angles are used (orange dashed) or half of the data points are considered (green dotted) for ^{208}Pb(n,n) at 30 MeV 95% confidence intervals and percentage uncertainty plot.

3.4.11 Bayesian approach to constrain parameters of the Equation of State

Participants: C.Y. Tsang (g), W.G. Lynch, M.B. Tsang

Description: Transport model theory predicts that ratios of neutron and proton energy spectra provide constraints on the density and momentum dependencies of the isovector mean-field potential. To extract the parameters of the equation of state, (ρ, S(ρ), m_n^*, m_p^* corresponding to density, symmetry energy, neutron and proton effective masses, respectively), we compare single and double n/p ratios obtained from central collisions of ^{112}Sn+^{112}Sn and ^{124}Sn+^{124}Sn at 120 MeV/u to a transport model calculations. Using Bayesian analysis which samples millions of parameter sets, we obtain the 1 and 2 sigma contours of the density dependence of the symmetry energy (see figure). For the effective mass, the results are more ambiguous. We need better data especially at higher kinetic energy where sensitivity to the effective mass splitting is larger.

FRIB relevance: Determining the nuclear equation of state is an important component of the FRIB science.

Outcomes: *Constraining the symmetry energy with heavy-ion collisions and Bayesian analyses*, P. Morfouace, C.Y. Tsang, Y.Zhang, W.G. Lynch, M.B.Tsang, et al., Phys. Lett. B 799 135045 (2019) .

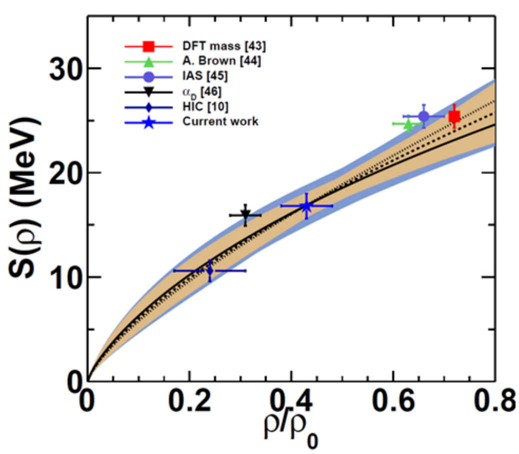

Figure 18: Density dependence of the symmetry energy S(ρ). The color areas correspond to the symmetry energy versus density of the 1σ (brown) and 2σ (blue) contours from Bayesian analysis of single and double ratios of central collisions of ^{112}Sn+^{112}Sn and ^{124}Sn+^{124}Sn at 120 MeV/u. Symbols are data from different experiments.

3.4.12 Bayesian approach to study the correlations of neutron star deformability and Equation of State parameters

Participants: C.Y. Tsang (g) and M.B. Tsang

Description: We use a Bayesian inference analysis to explore the sensitivity of Taylor expansion parameters of the nuclear equation of state (EOS) to the neutron star dimensionless tidal deformability (Λ) obtained from the neutron star merger event GW170817. To avoid correlations between the expansion parameters, we use a prior distributions based on a recently published meta-modeling approach. However, we find that assumptions in the prior distribution strongly influence the constraints on Λ. The sensitivity study is extended beyond the canonical neutron star with 1.4 solar mass. For neutron star with mass < 1.6 solar mass, L_{sym} and K_{sym} are highly correlated with the tidal deformability. For more massive neutron stars, the tidal deformability is more strongly correlated with higher order Taylor expansion parameters.

FRIB relevance: Investigating dense nuclear matter on earth and in heavens is one of the major objectives in FRIB science.

Outcomes: *Insights on Skyrme parameters from GW170817*, C. Y. Tsang, M. B. Tsang, P. Danielewicz, F. J. Fattoyev,and W. G. Lynch, Phys. Lett. B 796 1 (2019) .

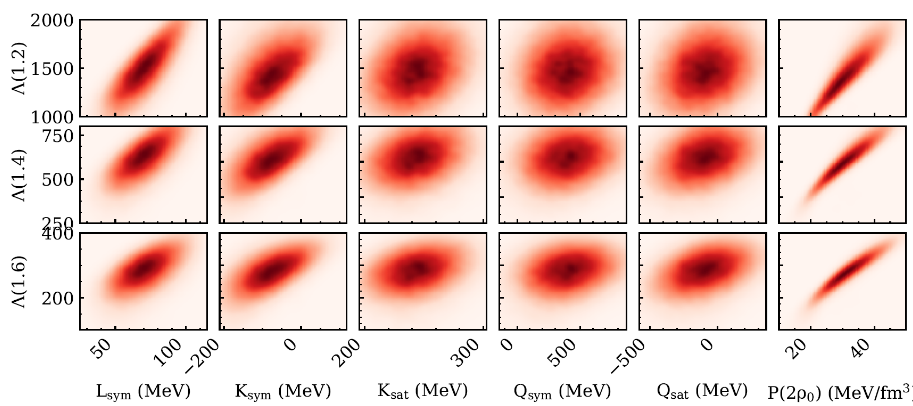

Figure 19: Bivariate distributions between neutron star deformabilities (Λ) and Taylor expansion parameters, L, K, Q and pressure at twice normal nuclear matter density, $P(2\rho_0)$ for neutron stars with different masses.

3.4.13 Applying Machine Learning to Bayesian Emulators

Participants: S. Pratt

Description: Equation-of-state analyses require rigorous comparison of large heterogeneous data sets to sophisticated models, using input from nuclear structure, heavy-ion collisions and astrophysical observations. Due to the numerical expense of theoretical models model emulators have been employed to explore the highly multi-dimensional model space. Emulators approximate the full model by interpolating from a modest number of full-model runs, but even with an emulator these studies push the limits of large computing facilities. For example, the Bayesian exploration summarized in the figure below involved 1200 full model runs over a 14-dimensional parameter space. One must choose how many full model runs to perform, and at which points, and with what accuracy. If the runs require a sampling of events, should one sample fewer events or use the computational budget to explore more points in parameter space. Machine learning provides a natural strategy for guiding and optimizing these studies. Such optimizations might save large amounts of computational expense, and make certain studies tenable that might otherwise be inconceivable.

FRIB relevance: Data from heavy-ion collisions and structure experiments from FRIB will both play a critical role in equation of state analyses.

Outcomes: S. Pratt, E. Sangaline, P. Sorensen and H. Wang, *Constraining the Eq. of State of Super-Hadronic Matter from Heavy-Ion Collisions*, Phys. Rev. Lett. **114**, 202301 (2015) .

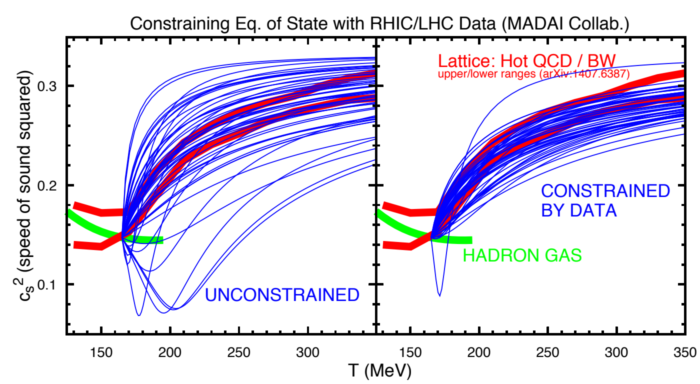

Figure 20: The equation of state derived from a 14-parameter Bayesian analysis. Eq.s of state from a random assortment of parameters (left panel, Bayesian prior) are compared to those weighted by the Bayesian likelihood(right panel).

3.4.14 Bayesian Inference of Symmetry Energy Characteristics from Nucleon Induced Reactions

Participants: P. Danielewicz

Description: Symmetry energy quantifies changes in the nuclear equation of state with changes in the neutron-proton imbalance. Knowledge of the symmetry energy as a function of density is essential for extrapolating from nuclear laboratory measurements to properties of neutron stars. The symmetry energy at saturation and subsaturation densities affects relative distribution of neutrons and protons in nuclei and isospin structure of the optical potential that governs nucleon elastic scattering and quasielastic charge exchange reactions. By simultaneously analyzing data from nucleon elastic scattering and nucleon quasielastic charge exchange reactions for the same targets and combining these analyses with results of other data on isospin characteristics of nuclei, in layers of Bayesian inference, Danielewicz et al. placed constraints on stiffness of the symmetry energy.

FRIB relevance: Inferences from measurements at FRIB, pertaining to the nuclear equation of state, need to be combined in a rational manner with inferences from data collected elsewhere, often in completely different measurements, and from astronomical observations.

Outcomes: P. Danielewicz, P. Singh and J. Lee, *Symmetry Energy III: Isovector Skins*, Nucl. Phys. A **958**, 147 (2017) .

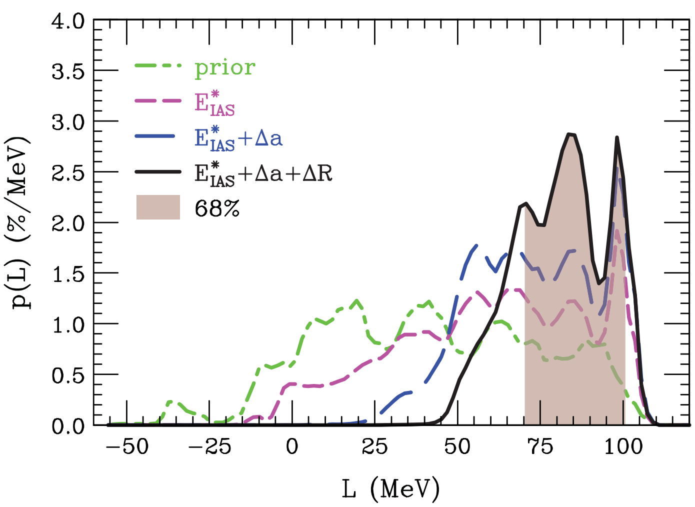

Figure 21: Evolution of likelihood for the stiffness of symmetry energy L as more data are taken into consideration.

4 Education and Workforce

There are only 26,000 AI researchers currently in the US. This is estimated to represent only a fifth of the current demand. There is an urgent need for training in AI, at a variety of educational levels and for diverse audiences. To this end, beyond our research efforts, we develop a range of outreach, recruitment, and educational activities. These activities will serve to raise interest in AI-related fields. We aim to retain talented students in AI-related fields and to help them to secure employment in a wide range of careers, thus ensuring that the new techniques and concepts developed at FRIB are widely disseminated.

- In order to develop education and training efforts that target AI and ML related methods applied to Nuclear Physics, in 2019 we organized a four day long FRIB-TA workshop on *ML methods in Nuclear physics* at NSCL/FRIB, with more than 100 participants.

- In 2020 several of us (Bazin, Hjorth-Jensen and Liddick) will teach a three-week long Nuclear Talent course at ECT* on Machine Learning and Data Analysis applied to nuclear physics.

- From spring 2020 (April and May, and planned to be repeated on an annual basis) we will host and run intensive courses on ML, Bayesian inference, and statistical data analysis for students and faculty in theoretical and experimental nuclear physics. The aim is to develop a large amount of material with lectures notes, videos, projects and hands-on material that can serve the whole nuclear Physics community. An example of possible material can found at . The format of the course is similar to a Nuclear TALENT course.

- We initiated the series of meetings on *Enhancing the interaction between nuclear experiment and theory through information and statistics* (ISNET). The next ISNET-8 will be held at FRIB during Dec. 14-17th, 2020.

5 Appendix: Anticipated projects

5.1 Detectors

5.1.1 Particle reconstruction of Time Projection Chamber

Participants: C.Y. Tsang (g), W.G. Lynch, M.B. Tsang

Description: To investigate the "nature of neutron-rich matter in the cosmos and on earth" is one of the scientific objectives laid out in the 2015 NSAC Long Range Plan. With the energy and the availability of rare isotope beams, FRIB and FRIB400 are poised to study the Equation of State of asymmetric matter. One observable to study the EoS is to compare the relative emission of members of isospin multiplets, e.g. π^- vs. π^+, n vs. p, t vs. ^{3}He, etc., which experience symmetry potentials and symmetry forces of opposite sign. Time projection chamber (TPC) provides large coverage to detect charged particles including pions emitted in heavy ion collisions (See figures). However, with mean multiplicity of 50 in the example shown, it becomes a challenge to reconstruct particle tracks, identify and accurately determine the momenta of the particles. We are looking into applying ML reconstruction algorithms pioneered in high energy physics.

FRIB relevance: The SpiRIT TPC (funded by DOE) will be moved from RIKEN to FRIB. When the TPC is placed inside the HRS, it will be the anchor detector for the Equation of State program at FRIB and FRIB400. Both online and offline analysis of TPC data will require fast and accurate reconstruction of the particle tracks.

Outcomes: None.

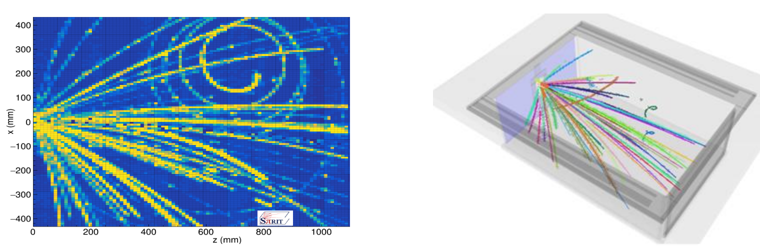

Figure 22: Tracks from two different events from $^{132}Sn +^{124} Sn$ collisions as viewed from the top (left panel) and 3D (right panel). The big spiral in the left panel is an emitted low energy π^-.

5.1.2 Particle ID for the NSCL/FRIB fragment separator

Participants: S. Schwarz, E. Kwan, M. Steiner, C. Sumithrarachchi, T. Ginter

Description: Rare-isotope experiments at the NSCL using fragmentation beams rely on the A1900 separator to isolate the reaction product of interest from background. An important tool to select and separate the correct particle are characteristic plots of energy loss in matter vs. time-of-flight, measured in relation to a fixed accelerator RF phase. Depending on beam and separator conditions, particles with a large number of different N, Z and charge states can contribute to the dE-ToF plots, turning particle ID into a challenge. Known patterns of particles with certain relations of N, Z and RF period, as well as energy-loss relations can be exploited for orientation. Complementary codes are being developed in order to assist and automate the particle-ID process. ML algorithms, e.g. ones popular for image matching, are being evaluated to map calculated plots, e.g. obtained with the LISE++ code, to the experimental ones.

FRIB relevance: Also at FRIB, a fragment separator will provide purified rare-isotope beams to users. Fast particle ID will become even more important to maximize precious beam time for users.

Outcomes: None.

5.2 Analysis of Final States

5.2.1 Multiparticle final states in central collisions

Participants: P. Nzabahimana (g), P. Danielewicz

Description: Central collisions of heavy nuclei serve as means of learning about bulk properties of nuclear matter at varying conditions of density, temperature and neutron-proton asymmetry, in the laboratory. These collisions further act as a black-body source yielding all products allowed by energy conservation and time scale for production, including unstable many-body states that decay in a variety of ways in the aftermath of the collision. Past development of strategies for extracting useful information from the mutiparticle final states of the collision was driven by intuitions but these do not stack up well against the vast amount of information nominally contained in the multiparticle measurements. The potential of AI techniques to access such information has been already demonstrated for ultrarelativistic collisions. Nzabahimanan and Danielewicz progress in applying AI to the multiparticle states at FRIB energies concentrating first on the identification of excited states with complicated decay patterns.

FRIB relevance: Central collisions will be studied at FRIB both to learn about the equation of state of nuclear matter and to study energies and nature of particle unstable excited states.

Outcomes: None .

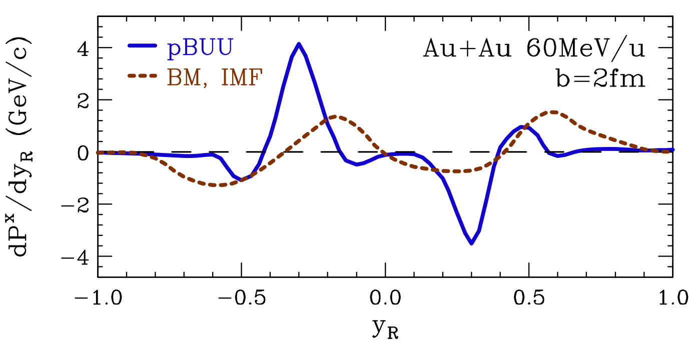

Figure 23: Differential flow of varying sign, predicted for central low-energy collisions in different models, will defy standard methods of flow detection in final-state analysis.